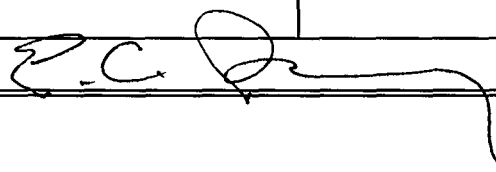


SOFTWARE RELEASE NOTICE

1. SRN Number: <b>G H G C - S R N - 130</b>		
2. Project Title: <b>Near-field environment I&amp;T1</b>		Project No. <b>20-1402-562</b>
3. SRN Title: <b>MULTIFLO Version 1.0</b>		
4. Originator/Requestor: <b>Scott Painter</b>		Date: <b>December 29, 1999</b> <b>San</b>
5. Summary of Actions  <input type="checkbox"/> Release of new software  <input type="checkbox"/> Release of modified software:  <input type="checkbox"/> Enhancements made  <input type="checkbox"/> Corrections made  <input type="checkbox"/> Change of access software  <input checked="" type="checkbox"/> Software Retirement		
6. Persons Authorized Access		
Name	Read Only/Read-Write	Addition/Change/Delete
7. Element Manager Approval: <b>Shelton for ECP</b>		Date: <b>12/29/99</b>
8. Remarks:  <b>Superseded by Version 1.2 b</b>		


8/78

# SOFTWARE RELEASE NOTICE

01. SRN Number: GHGC-SRN-130		
02. Project Title: Near-Field Environment KTI		Project No. 20-5708-562
03. SRN Title: MULTIFLO Version 1.0		
04. Originator/Requestor: Bruce Mabrito		Date: 04/07/97
05. Summary of Actions <ul style="list-style-type: none"> <li><input checked="" type="checkbox"/> Release of new software</li> <li><input type="checkbox"/> Release of modified software:             <ul style="list-style-type: none"> <li><input type="checkbox"/> Enhancements made</li> <li><input type="checkbox"/> Corrections made</li> </ul> </li> <li><input type="checkbox"/> Change of access software</li> <li><input type="checkbox"/> Software Retirement</li> </ul>		
06. Persons Authorized Access		
Name	RO/RW	A/C/D
Peter C. Lichtner	RW	
Mohan Seth	RW	
Narasi Sridhar	RO	
Brett Leslie	RO	
English Percy	RO	
07. Element Manager Approval: 		Date: 4/7/97
08. Remarks:		

9/79

## SOFTWARE SUMMARY FORM

01. Summary Date: 04/07/97	02. Summary prepared by (Name and phone) Peter C. Lichtner, 522-6084	03. Summary Action:  New	
04. Software Date: 04/04/97	05. Short Title: MULTIFLO Version 1.0		
06. Software Title:  MULTIFLO Version 1.0		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:  Peter Lichtner, (210) 522-6084 Mohan Seth, (972) 699-3610	
13. Narrative: The code is used to model multiphase groundwater flow and reactive transport.			
14. Computer Platform  SUN	15. Computer Operating System:  UNIX	16. Programming Language(s):  Fortran 77	17. Number of Source Program Statements:  ~ 64,000
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	
Software Custodian: <u></u> Date: <u>4/7/97</u>			

F - QA records. 13/79  
4/14/87 Peter Lichten

## RELEASE NOTES (4/11/97)

This is a preliminary release of the software package MULTIFLO, Version 1.0, dated February, 1997. This version is NOT to be used in any official capacity, but only for the purposes of instructional use of the code. The results produced by this preliminary version are known to differ from the most recent version of the code (Version 1.0, April, 1997) which is considered to be more reliable. Furthermore, several options listed in the manual as detailed below are not available with the preliminary release version.

The following restrictions supercede the manual and apply to the preliminary release, Version 1.0 of MULTIFLO, dated February, 1997. There are known bugs in this release which prohibit its use for serious work. However, the February version contains most of the options available in the April release, and as such, can be used for learning how to use the code.

- 0) In the COMP and BCON keywords it is not possible to specify the region over which the initial or boundary condition applies. In the preliminary release version they are assumed to apply uniformly over the entire domain. Omit the input data over the region and the zero closing the block of data. Refer to the original MULTIFLO manual, Part II: MULTIFLO 1.0 and GEM 1.0, for details.
- 1) Explicit and operator splitting methods (METHOD = 2 & 3) apply only to a pure liquid fully saturated system.
- 2) If using the operator splitting algorithm for a transport problem involving only homogeneous reactions, it is only possible to obtain the total primary concentrations and not the individual species concentrations in the plot files.
- 3) The electrochemical migration option in GEM (MODE = 1) is not available in the present release. Equal diffusion coefficients are used for all species as specified in the DIFF keyword.
- 4) It is not possible in the current version of MULTIFLO to model a system in which all or part of the system constitutes a pure gas phase. A liquid phase must always be present. A pure liquid phase, however, is possible to model.
- 5) Ion-exchange is only functional for the implicit finite difference algorithm (METHOD = 1). The selectivity coefficients are constants independent of temperature.
- 6) Dispersion is not incorporated in the current version of the code. It is recommended to use heterogeneous media rather than dispersion coefficients.
- 7) In the fully implicit time stepping algorithm, the Courant number does not limit the time step size.

14/79

rwxr-xr-x	0/1	0 Apr	4 16:47 1997	multiflo/
rwxr-xr-x	0/1	0 Apr	4 16:57 1997	multiflo/metra/
r--r--r--	0/1	1085 Apr	4 16:57 1997	multiflo/metra/pckr.h
r--r--r--	0/1	16133 Apr	4 16:56 1997	multiflo/metra/accm.f
r--r--r--	0/1	1794 Apr	4 16:57 1997	multiflo/metra/paramtrs.h
r--r--r--	0/1	16257 Apr	4 16:56 1997	multiflo/metra/accmvp.f
rwxr-xr-x	0/1	0 Apr	4 16:58 1997	multiflo/metra/SCCS/
r--r--r--	0/1	16384 Apr	4 16:58 1997	multiflo/metra/SCCS/s.accm.f
r--r--r--	0/1	16508 Apr	4 16:58 1997	multiflo/metra/SCCS/s.accmvp.f
r--r--r--	0/1	15553 Apr	4 16:58 1997	multiflo/metra/SCCS/s.allot.f
r--r--r--	0/1	24763 Apr	4 16:58 1997	multiflo/metra/SCCS/s.bcond.f
r--r--r--	0/1	8170 Apr	4 16:58 1997	multiflo/metra/SCCS/s.blkdtmet.f
r--r--r--	0/1	28994 Apr	4 16:58 1997	multiflo/metra/SCCS/s.coefs.f
r--r--r--	0/1	30149 Apr	4 16:58 1997	multiflo/metra/SCCS/s.coefsvp.f
r--r--r--	0/1	37545 Apr	4 16:58 1997	multiflo/metra/SCCS/s.cond.f
r--r--r--	0/1	46542 Apr	4 16:58 1997	multiflo/metra/SCCS/s.d4gaus.f
r--r--r--	0/1	7501 Apr	4 16:58 1997	multiflo/metra/SCCS/s.debug.f
r--r--r--	0/1	18020 Apr	4 16:58 1997	multiflo/metra/SCCS/s.dtstep.f
r--r--r--	0/1	21362 Apr	4 16:58 1997	multiflo/metra/SCCS/s.ecmtbl.f
r--r--r--	0/1	19438 Apr	4 16:58 1997	multiflo/metra/SCCS/s.emip.f
r--r--r--	0/1	18419 Apr	4 16:58 1997	multiflo/metra/SCCS/s.equil.f
r--r--r--	0/1	12152 Apr	4 16:58 1997	multiflo/metra/SCCS/s.griddat.f
r--r--r--	0/1	55931 Apr	4 16:58 1997	multiflo/metra/SCCS/s.init.f
r--r--r--	0/1	47101 Apr	4 16:58 1997	multiflo/metra/SCCS/s.inpmetra.f
r--r--r--	0/1	23521 Apr	4 16:58 1997	multiflo/metra/SCCS/s.iter.f
r--r--r--	0/1	39899 Apr	4 16:58 1997	multiflo/metra/SCCS/s.mainmetra.f
r--r--r--	0/1	364 Apr	4 16:58 1997	multiflo/metra/SCCS/s.misc.f
r--r--r--	0/1	15026 Apr	4 16:58 1997	multiflo/metra/SCCS/s.openfls.f
r--r--r--	0/1	28063 Apr	4 16:58 1997	multiflo/metra/SCCS/s.outmetra.f
r--r--r--	0/1	23907 Apr	4 16:58 1997	multiflo/metra/SCCS/s.pckr.f
r--r--r--	0/1	35621 Apr	4 16:58 1997	multiflo/metra/SCCS/s.plots.f
r--r--r--	0/1	12057 Apr	4 16:58 1997	multiflo/metra/SCCS/s.prints.f
r--r--r--	0/1	26987 Apr	4 16:58 1997	multiflo/metra/SCCS/s.pvt.f
r--r--r--	0/1	19213 Apr	4 16:58 1997	multiflo/metra/SCCS/s.pvtfunc.f
r--r--r--	0/1	28979 Apr	4 16:58 1997	multiflo/metra/SCCS/s.pvth2o.f
r--r--r--	0/1	25909 Apr	4 16:58 1997	multiflo/metra/SCCS/s.pvtvp.f
r--r--r--	0/1	53547 Apr	4 16:58 1997	multiflo/metra/SCCS/s.recdat.f
r--r--r--	0/1	16112 Apr	4 16:58 1997	multiflo/metra/SCCS/s.rstart.f
r--r--r--	0/1	12371 Apr	4 16:58 1997	multiflo/metra/SCCS/s.setbc.f
r--r--r--	0/1	20177 Apr	4 16:58 1997	multiflo/metra/SCCS/s.slvliq.f
r--r--r--	0/1	11771 Apr	4 16:58 1997	multiflo/metra/SCCS/s.solve.f
r--r--r--	0/1	15608 Apr	4 16:58 1997	multiflo/metra/SCCS/s.source.f
r--r--r--	0/1	12918 Apr	4 16:58 1997	multiflo/metra/SCCS/s.thomas.f
r--r--r--	0/1	16752 Apr	4 16:58 1997	multiflo/metra/SCCS/s.trans.f
r--r--r--	0/1	8717 Apr	4 16:58 1997	multiflo/metra/SCCS/s.update.f
r--r--r--	0/1	15355 Apr	4 16:58 1997	multiflo/metra/SCCS/s.updtpsk.f
r--r--r--	0/1	16539 Apr	4 16:58 1997	multiflo/metra/SCCS/s.updtpk.f
r--r--r--	0/1	50852 Apr	4 16:58 1997	multiflo/metra/SCCS/s.watsolv.f
r--r--r--	0/1	2740 Apr	4 16:57 1997	multiflo/metra/SCCS/s.add.h
r--r--r--	0/1	5385 Apr	4 16:57 1997	multiflo/metra/SCCS/s.com.h
r--r--r--	0/1	884 Apr	4 16:58 1997	multiflo/metra/SCCS/s.frfmt.h
r--r--r--	0/1	640 Apr	4 16:58 1997	multiflo/metra/SCCS/s.impl.h
r--r--r--	0/1	1209 Apr	4 16:58 1997	multiflo/metra/SCCS/s.metragem.h
r--r--r--	0/1	2045 Apr	4 16:58 1997	multiflo/metra/SCCS/s.paramtrs.h
r--r--r--	0/1	1336 Apr	4 16:58 1997	multiflo/metra/SCCS/s.pckr.h
r--r--r--	0/1	816 Apr	4 16:58 1997	multiflo/metra/SCCS/s.pvtfunc.h
r--r--r--	0/1	1167 Apr	4 16:58 1997	multiflo/metra/SCCS/s.pvttbl.h
r--r--r--	0/1	1816 Apr	4 16:58 1997	multiflo/metra/SCCS/s.scalars.h
r--r--r--	0/1	511 Apr	4 16:58 1997	multiflo/metra/SCCS/s.units.h
r--r--r--	0/1	639 Apr	4 16:58 1997	multiflo/metra/SCCS/s.watsolv.h

MULTIFLO V1.0  
4 APR 97

1/8

15/79

```

r--r--r-- 0/1 3761 Apr 4 16:58 1997 multiflo/metra/SCCS/s.Makefile
r--r--r-- 0/1 15302 Apr 4 16:56 1997 multiflo/metra/allot.f
r--r--r-- 0/1 24512 Apr 4 16:56 1997 multiflo/metra/bcond.f
r--r--r-- 0/1 7919 Apr 4 16:56 1997 multiflo/metra/blkdtmet.f
r--r--r-- 0/1 28743 Apr 4 16:56 1997 multiflo/metra/coefs.f
r--r--r-- 0/1 29898 Apr 4 16:56 1997 multiflo/metra/coefsvp.f
r--r--r-- 0/1 37294 Apr 4 16:56 1997 multiflo/metra/cond.f
r--r--r-- 0/1 46291 Apr 4 16:57 1997 multiflo/metra/d4gaus.f
r--r--r-- 0/1 7250 Apr 4 16:57 1997 multiflo/metra/debug.f
r--r--r-- 0/1 17769 Apr 4 16:57 1997 multiflo/metra/dtstep.f
r--r--r-- 0/1 21111 Apr 4 16:57 1997 multiflo/metra/ecmtbl.f
r--r--r-- 0/1 19187 Apr 4 16:57 1997 multiflo/metra/emip.f
r--r--r-- 0/1 18168 Apr 4 16:57 1997 multiflo/metra/equil.f
r--r--r-- 0/1 11901 Apr 4 16:57 1997 multiflo/metra/griddat.f
r--r--r-- 0/1 55680 Apr 4 16:57 1997 multiflo/metra/init.f
r--r--r-- 0/1 23270 Apr 4 16:57 1997 multiflo/metra/iter.f
rwxr-xr-x 0/1 504 Mar 11 13:53 1997 multiflo/metra/cat_metra
r--r--r-- 0/1 46850 Apr 4 16:57 1997 multiflo/metra/inpmetra.f
r--r--r-- 0/1 39648 Apr 4 16:57 1997 multiflo/metra/mainmetra.f
r--r--r-- 0/1 113 Apr 4 16:57 1997 multiflo/metra/misc.f
r--r--r-- 0/1 14775 Apr 4 16:57 1997 multiflo/metra/openfls.f
r--r--r-- 0/1 27812 Apr 4 16:57 1997 multiflo/metra/outmetra.f
r--r--r-- 0/1 23656 Apr 4 16:57 1997 multiflo/metra/pckr.f
r--r--r-- 0/1 35370 Apr 4 16:57 1997 multiflo/metra/plots.f
r--r--r-- 0/1 11806 Apr 4 16:57 1997 multiflo/metra/prints.f
r--r--r-- 0/1 26736 Apr 4 16:57 1997 multiflo/metra/pvt.f
r--r--r-- 0/1 18962 Apr 4 16:57 1997 multiflo/metra/pvtfunc.f
r--r--r-- 0/1 28728 Apr 4 16:57 1997 multiflo/metra/pvth2o.f
r--r--r-- 0/1 25658 Apr 4 16:57 1997 multiflo/metra/pvtvp.f
r--r--r-- 0/1 53296 Apr 4 16:57 1997 multiflo/metra/reccdat.f
r--r--r-- 0/1 15861 Apr 4 16:57 1997 multiflo/metra/rstart.f
r--r--r-- 0/1 12120 Apr 4 16:57 1997 multiflo/metra/setbc.f
r--r--r-- 0/1 19926 Apr 4 16:57 1997 multiflo/metra/slvliq.f
r--r--r-- 0/1 11520 Apr 4 16:57 1997 multiflo/metra/solve.f
rw-r--r-- 0/1 90226 Dec 19 10:26 1995 multiflo/metra/.dir.tiff
r--r--r-- 0/1 15357 Apr 4 16:57 1997 multiflo/metra/source.f
r--r--r-- 0/1 16501 Apr 4 16:57 1997 multiflo/metra/trans.f
rw-r--r-- 0/1 943456 Mar 6 09:23 1997 multiflo/metra/metramaster.for
rwxr-xr-x 0/1 0 Apr 4 16:55 1997 multiflo/metra/bin/
rw-r--r-- 0/1 9716 Apr 3 11:48 1997 multiflo/metra/bin/accm.o
rw-r--r-- 0/1 11024 Apr 3 11:48 1997 multiflo/metra/bin/accmvp.o
rw-r--r-- 0/1 8660 Apr 3 11:48 1997 multiflo/metra/bin/allot.o
rw-r--r-- 0/1 14032 Apr 3 11:48 1997 multiflo/metra/bin/bcond.o
rw-r--r-- 0/1 241684 Apr 3 11:48 1997 multiflo/metra/bin/blkdtmet.o
rw-r--r-- 0/1 18892 Apr 3 11:48 1997 multiflo/metra/bin/coefs.o
rw-r--r-- 0/1 20616 Apr 3 11:49 1997 multiflo/metra/bin/coefsvp.o
rw-r--r-- 0/1 24896 Apr 3 11:49 1997 multiflo/metra/bin/cond.o
rw-r--r-- 0/1 24484 Apr 3 11:49 1997 multiflo/metra/bin/d4gaus.o
rw-r--r-- 0/1 5480 Apr 3 11:49 1997 multiflo/metra/bin/debug.o
rw-r--r-- 0/1 3988 Apr 3 11:48 1997 multiflo/metra/bin/dtstep.o
rw-r--r-- 0/1 15608 Apr 3 11:49 1997 multiflo/metra/bin/ecmtbl.o
rw-r--r-- 0/1 19880 Apr 3 11:49 1997 multiflo/metra/bin/emip.o
rw-r--r-- 0/1 12280 Apr 3 11:50 1997 multiflo/metra/bin/equil.o
rw-r--r-- 0/1 8432 Apr 3 11:50 1997 multiflo/metra/bin/griddat.o
rw-r--r-- 0/1 71052 Apr 3 11:50 1997 multiflo/metra/bin/init.o
rw-r--r-- 0/1 81088 Apr 3 11:51 1997 multiflo/metra/bin/inpmetra.o
rw-r--r-- 0/1 19696 Apr 3 11:51 1997 multiflo/metra/bin/iter.o
rw-r--r-- 0/1 32472 Apr 3 11:48 1997 multiflo/metra/bin/mainmetra.o
rw-r--r-- 0/1 7236 Apr 3 11:51 1997 multiflo/metra/bin/openfls.o
rw-r--r-- 0/1 41368 Apr 3 11:51 1997 multiflo/metra/bin/outmetra.o

```

2/8

rw-r--r--	0/1	13992	Apr	3	11:51	1997	mul	co/metra/bin/pckr.o
rw-r--r--	0/1	119272	Apr	3	11:52	1997	multiflo	metra/bin/plots.o
rw-r--r--	0/1	18784	Apr	3	11:52	1997	multiflo	metra/bin/prints.o
rw-r--r--	0/1	22928	Apr	3	11:52	1997	multiflo	metra/bin/pvt.o
rw-r--r--	0/1	13452	Apr	3	11:53	1997	multiflo	metra/bin/pvtfunc.o
rw-r--r--	0/1	26348	Apr	3	11:53	1997	multiflo	metra/bin/pvth2o.o
rw-r--r--	0/1	22800	Apr	3	11:53	1997	multiflo	metra/bin/pvtvp.o
rw-r--r--	0/1	75900	Apr	3	11:54	1997	multiflo	metra/bin/reccdat.o
rw-r--r--	0/1	33936	Apr	3	11:55	1997	multiflo	metra/bin/rstart.o
rw-r--r--	0/1	8168	Apr	3	11:55	1997	multiflo	metra/bin/setbc.o
rw-r--r--	0/1	18732	Apr	3	11:55	1997	multiflo	metra/bin/slvliq.o
rw-r--r--	0/1	4812	Apr	3	11:55	1997	multiflo	metra/bin/solve.o
rw-r--r--	0/1	11204	Apr	3	11:55	1997	multiflo	metra/bin/source.o
rw-r--r--	0/1	5876	Apr	3	11:55	1997	multiflo	metra/bin/thomas.o
rw-r--r--	0/1	10900	Apr	3	11:55	1997	multiflo	metra/bin/trans.o
rw-r--r--	0/1	3156	Apr	3	11:55	1997	multiflo	metra/bin/update.o
rw-r--r--	0/1	9140	Apr	3	11:55	1997	multiflo	metra/bin/updtpsk.o
rw-r--r--	0/1	11632	Apr	3	11:56	1997	multiflo	metra/bin/updtvpk.o
rw-r--r--	0/1	55444	Apr	3	11:57	1997	multiflo	metra/bin/watsolv.o
rw-r--r--	0/1	1081344	Apr	3	11:57	1997	multiflo	metra/bin/metra
r--r--r--	0/1	12667	Apr	4	16:57	1997	multiflo	metra/thomas.f
r--r--r--	0/1	8466	Apr	4	16:57	1997	multiflo	metra/update.f
r--r--r--	0/1	15104	Apr	4	16:57	1997	multiflo	metra/updtpsk.f
r--r--r--	0/1	16288	Apr	4	16:57	1997	multiflo	metra/updtvpk.f
r--r--r--	0/1	50601	Apr	4	16:57	1997	multiflo	metra/watsolv.f
r--r--r--	0/1	2489	Apr	4	16:57	1997	multiflo	metra/add.h
r--r--r--	0/1	5134	Apr	4	16:57	1997	multiflo	metra/com.h
r--r--r--	0/1	633	Apr	4	16:57	1997	multiflo	metra/frfmt.h
r--r--r--	0/1	389	Apr	4	16:57	1997	multiflo	metra/impl.h
r--r--r--	0/1	958	Apr	4	16:57	1997	multiflo	metra/metragem.h
r--r--r--	0/1	565	Apr	4	16:57	1997	multiflo	metra/pvtfunc.h
r--r--r--	0/1	916	Apr	4	16:57	1997	multiflo	metra/pvttbl.h
r--r--r--	0/1	1565	Apr	4	16:57	1997	multiflo	metra/scalars.h
r--r--r--	0/1	260	Apr	4	16:57	1997	multiflo	metra/units.h
r--r--r--	0/1	388	Apr	4	16:57	1997	multiflo	metra/watsolv.h
r--r--r--	0/1	3510	Apr	4	16:57	1997	multiflo	metra/Makefile
rw-r--r--	0/1	0	Apr	4	16:54	1997	multiflo	gem/
r--r--r--	0/1	16546	Apr	4	16:50	1997	multiflo	gem/allotgem.f
rw-r--r--	0/1	0	Apr	4	16:52	1997	multiflo	gem/SCCS/
r--r--r--	0/1	16797	Apr	4	16:51	1997	multiflo	gem/SCCS/s.allotgem.f
r--r--r--	0/1	5249	Apr	4	16:51	1997	multiflo	gem/SCCS/s.blkdtgem.f
r--r--r--	0/1	10450	Apr	4	16:51	1997	multiflo	gem/SCCS/s.bndcond.f
r--r--r--	0/1	13598	Apr	4	16:51	1997	multiflo	gem/SCCS/s.cehyliq.f
r--r--r--	0/1	21142	Apr	4	16:51	1997	multiflo	gem/SCCS/s.cehytwp.f
r--r--r--	0/1	16445	Apr	4	16:51	1997	multiflo	gem/SCCS/s.cetvdlq.f
r--r--r--	0/1	26646	Apr	4	16:51	1997	multiflo	gem/SCCS/s.cetvdtwp.f
r--r--r--	0/1	5129	Apr	4	16:51	1997	multiflo	gem/SCCS/s.cexact.f
r--r--r--	0/1	14116	Apr	4	16:51	1997	multiflo	gem/SCCS/s.cgasos.f
r--r--r--	0/1	21334	Apr	4	16:51	1997	multiflo	gem/SCCS/s.cihytwp.f
r--r--r--	0/1	14378	Apr	4	16:51	1997	multiflo	gem/SCCS/s.cliqos.f
r--r--r--	0/1	13271	Apr	4	16:51	1997	multiflo	gem/SCCS/s.coefrxn.f
r--r--r--	0/1	14450	Apr	4	16:51	1997	multiflo	gem/SCCS/s.coshyliq.f
r--r--r--	0/1	12224	Apr	4	16:51	1997	multiflo	gem/SCCS/s.dataall.f
r--r--r--	0/1	34770	Apr	4	16:51	1997	multiflo	gem/SCCS/s.database.f
r--r--r--	0/1	6160	Apr	4	16:51	1997	multiflo	gem/SCCS/s.density.f
r--r--r--	0/1	6418	Apr	4	16:51	1997	multiflo	gem/SCCS/s.difoft.f
r--r--r--	0/1	10913	Apr	4	16:51	1997	multiflo	gem/SCCS/s.eqjac.f
r--r--r--	0/1	13278	Apr	4	16:51	1997	multiflo	gem/SCCS/s.eqlib.f
r--r--r--	0/1	10866	Apr	4	16:51	1997	multiflo	gem/SCCS/s.eqres.f
r--r--r--	0/1	12181	Apr	4	16:51	1997	multiflo	gem/SCCS/s.explicit.f

17/79

r--r--r--	0/1	5799	Apr	4	16:51	1997	mu	lo/gem/SCCS/s.fit.f
r--r--r--	0/1	4694	Apr	4	16:51	1997	multiflo/gem/SCCS/s.fkinet.f	
r--r--r--	0/1	4677	Apr	4	16:51	1997	multiflo/gem/SCCS/s.flogk.f	
r--r--r--	0/1	10384	Apr	4	16:51	1997	multiflo/gem/SCCS/s.fun.f	
r--r--r--	0/1	9841	Apr	4	16:51	1997	multiflo/gem/SCCS/s.gameq.f	
r--r--r--	0/1	8981	Apr	4	16:51	1997	multiflo/gem/SCCS/s.gamextd.f	
r--r--r--	0/1	11355	Apr	4	16:51	1997	multiflo/gem/SCCS/s.ghostpsi.f	
r--r--r--	0/1	18637	Apr	4	16:51	1997	multiflo/gem/SCCS/s.graph1d.f	
r--r--r--	0/1	21026	Apr	4	16:51	1997	multiflo/gem/SCCS/s.graph2d.f	
r--r--r--	0/1	16535	Apr	4	16:51	1997	multiflo/gem/SCCS/s.graph3d.f	
r--r--r--	0/1	9549	Apr	4	16:51	1997	multiflo/gem/SCCS/s.grid.f	
r--r--r--	0/1	10692	Apr	4	16:51	1997	multiflo/gem/SCCS/s.grid1d.f	
r--r--r--	0/1	10317	Apr	4	16:51	1997	multiflo/gem/SCCS/s.gunits.f	
r--r--r--	0/1	20725	Apr	4	16:51	1997	multiflo/gem/SCCS/s.hybrid.f	
r--r--r--	0/1	37532	Apr	4	16:51	1997	multiflo/gem/SCCS/s.initgem.f	
r--r--r--	0/1	9511	Apr	4	16:51	1997	multiflo/gem/SCCS/s.inirate.f	
r--r--r--	0/1	8830	Apr	4	16:51	1997	multiflo/gem/SCCS/s.interpf.f	
r--r--r--	0/1	7513	Apr	4	16:51	1997	multiflo/gem/SCCS/s.ionexc.f	
r--r--r--	0/1	9637	Apr	4	16:51	1997	multiflo/gem/SCCS/s.kinrxn.f	
r--r--r--	0/1	9874	Apr	4	16:51	1997	multiflo/gem/SCCS/s.kinrxn_orig.f	
r--r--r--	0/1	9058	Apr	4	16:51	1997	multiflo/gem/SCCS/s.kinrxnex.f	
r--r--r--	0/1	4833	Apr	4	16:51	1997	multiflo/gem/SCCS/s.lubksb.f	
r--r--r--	0/1	5698	Apr	4	16:51	1997	multiflo/gem/SCCS/s.ludcmp.f	
r--r--r--	0/1	36153	Apr	4	16:51	1997	multiflo/gem/SCCS/s.maingem.f	
r--r--r--	0/1	6497	Apr	4	16:51	1997	multiflo/gem/SCCS/s.massbal.f	
r--r--r--	0/1	323	Apr	4	16:51	1997	multiflo/gem/SCCS/s.gas.h	
r--r--r--	0/1	7217	Apr	4	16:51	1997	multiflo/gem/SCCS/s.mastrnex.f	
r--r--r--	0/1	7856	Apr	4	16:51	1997	multiflo/gem/SCCS/s.mastrnim.f	
r--r--r--	0/1	8245	Apr	4	16:51	1997	multiflo/gem/SCCS/s.mastrnos.f	
r--r--r--	0/1	5489	Apr	4	16:51	1997	multiflo/gem/SCCS/s.maxchg.f	
r--r--r--	0/1	9644	Apr	4	16:51	1997	multiflo/gem/SCCS/s.mltpsiex.f	
r--r--r--	0/1	7011	Apr	4	16:51	1997	multiflo/gem/SCCS/s.modbnd.f	
r--r--r--	0/1	4683	Apr	4	16:51	1997	multiflo/gem/SCCS/s.mprove.f	
r--r--r--	0/1	8699	Apr	4	16:51	1997	multiflo/gem/SCCS/s.opspltex.f	
r--r--r--	0/1	15228	Apr	4	16:51	1997	multiflo/gem/SCCS/s.opspltgl.f	
r--r--r--	0/1	7396	Apr	4	16:51	1997	multiflo/gem/SCCS/s.opspltim.f	
r--r--r--	0/1	22535	Apr	4	16:51	1997	multiflo/gem/SCCS/s.output1.f	
r--r--r--	0/1	21435	Apr	4	16:51	1997	multiflo/gem/SCCS/s.output2.f	
r--r--r--	0/1	37210	Apr	4	16:51	1997	multiflo/gem/SCCS/s.path.f	
r--r--r--	0/1	15333	Apr	4	16:51	1997	multiflo/gem/SCCS/s.pecletnr.f	
r--r--r--	0/1	5095	Apr	4	16:52	1997	multiflo/gem/SCCS/s.psat.f	
r--r--r--	0/1	61525	Apr	4	16:52	1997	multiflo/gem/SCCS/s.readat.f	
r--r--r--	0/1	7086	Apr	4	16:52	1997	multiflo/gem/SCCS/s.solprd.f	
r--r--r--	0/1	9157	Apr	4	16:52	1997	multiflo/gem/SCCS/s.solprodt.f	
r--r--r--	0/1	23427	Apr	4	16:52	1997	multiflo/gem/SCCS/s.solver.f	
r--r--r--	0/1	8824	Apr	4	16:52	1997	multiflo/gem/SCCS/s.speciate.f	
r--r--r--	0/1	15569	Apr	4	16:52	1997	multiflo/gem/SCCS/s.startup.f	
r--r--r--	0/1	11081	Apr	4	16:52	1997	multiflo/gem/SCCS/s.stdyst.f	
r--r--r--	0/1	7222	Apr	4	16:52	1997	multiflo/gem/SCCS/s.stepgem.f	
r--r--r--	0/1	13037	Apr	4	16:52	1997	multiflo/gem/SCCS/s.testgem.f	
r--r--r--	0/1	8136	Apr	4	16:52	1997	multiflo/gem/SCCS/s.textab.f	
r--r--r--	0/1	9785	Apr	4	16:52	1997	multiflo/gem/SCCS/s.transp.f	
r--r--r--	0/1	6505	Apr	4	16:52	1997	multiflo/gem/SCCS/s.unitconv.f	
r--r--r--	0/1	25074	Apr	4	16:52	1997	multiflo/gem/SCCS/s.updtgem.f	
r--r--r--	0/1	50869	Apr	4	16:52	1997	multiflo/gem/SCCS/s.watsolv.f	
r--r--r--	0/1	6138	Apr	4	16:52	1997	multiflo/gem/SCCS/s.zonek.f	
r--r--r--	0/1	1537	Apr	4	16:51	1997	multiflo/gem/SCCS/s.addgem.h	
r--r--r--	0/1	3736	Apr	4	16:51	1997	multiflo/gem/SCCS/s.comgem.h	
r--r--r--	0/1	570	Apr	4	16:51	1997	multiflo/gem/SCCS/s.cxkin.h	
r--r--r--	0/1	392	Apr	4	16:51	1997	multiflo/gem/SCCS/s.debye.h	



18/79

r--r--r--	0/1	546	Apr	4	16:51	1997	multiflo/gem/SCCS/s.fields.h
r--r--r--	0/1	754	Apr	4	16:51	1997	multiflo/gem/SCCS/s.frfmt.h
r--r--r--	0/1	430	Apr	4	16:51	1997	multiflo/gem/SCCS/s.impl.h
r--r--r--	0/1	408	Apr	4	16:51	1997	multiflo/gem/SCCS/s.iounits.h
r--r--r--	0/1	588	Apr	4	16:51	1997	multiflo/gem/SCCS/s.kinetic.h
r--r--r--	0/1	1209	Apr	4	16:51	1997	multiflo/gem/SCCS/s.metrage.h
r--r--r--	0/1	337	Apr	4	16:51	1997	multiflo/gem/SCCS/s.minrl.h
r--r--r--	0/1	767	Apr	4	16:51	1997	multiflo/gem/SCCS/s.ofiles.h
r--r--r--	0/1	2045	Apr	4	16:51	1997	multiflo/gem/SCCS/s.paramtrs.h
r--r--r--	0/1	1305	Apr	4	16:51	1997	multiflo/gem/SCCS/s.scalgem.h
r--r--r--	0/1	522	Apr	4	16:51	1997	multiflo/gem/SCCS/s.scratch.h
r--r--r--	0/1	605	Apr	4	16:51	1997	multiflo/gem/SCCS/s.surfkin.h
r--r--r--	0/1	319	Apr	4	16:51	1997	multiflo/gem/SCCS/s.tempfld.h
r--r--r--	0/1	314	Apr	4	16:51	1997	multiflo/gem/SCCS/s.velsat.h
r--r--r--	0/1	527	Apr	4	16:51	1997	multiflo/gem/SCCS/s.watsolv.h
r--r--r--	0/1	1492	Apr	4	16:52	1997	multiflo/gem/SCCS/s.Makefile
r--r--r--	0/1	5887	Apr	4	16:50	1997	multiflo/gem/zonek.f
r--r--r--	0/1	10662	Apr	4	16:50	1997	multiflo/gem/eqjac.f
r--r--r--	0/1	13027	Apr	4	16:50	1997	multiflo/gem/eqlib.f
r--r--r--	0/1	10615	Apr	4	16:50	1997	multiflo/gem/eqres.f
r--r--r--	0/1	5548	Apr	4	16:50	1997	multiflo/gem/fit.f
rwxr--r--	0/1	979	Mar	27	09:58	1997	multiflo/gem/cat_gem
r--r--r--	0/1	4998	Apr	4	16:50	1997	multiflo/gem/blkdtgem.f
r--r--r--	0/1	10199	Apr	4	16:50	1997	multiflo/gem/bndcond.f
r--r--r--	0/1	13347	Apr	4	16:50	1997	multiflo/gem/cehyliq.f
r--r--r--	0/1	20891	Apr	4	16:50	1997	multiflo/gem/cehytwpf.f
r--r--r--	0/1	16194	Apr	4	16:50	1997	multiflo/gem/cetvdlq.f
r--r--r--	0/1	26395	Apr	4	16:50	1997	multiflo/gem/cetvdtwp.f
r--r--r--	0/1	4878	Apr	4	16:50	1997	multiflo/gem/cexact.f
r--r--r--	0/1	13865	Apr	4	16:50	1997	multiflo/gem/cgasos.f
r--r--r--	0/1	21083	Apr	4	16:50	1997	multiflo/gem/cihytwpf.f
r--r--r--	0/1	14127	Apr	4	16:50	1997	multiflo/gem/cliqos.f
r--r--r--	0/1	13020	Apr	4	16:50	1997	multiflo/gem/coefrxn.f
r--r--r--	0/1	14199	Apr	4	16:50	1997	multiflo/gem/coshyliq.f
r--r--r--	0/1	11973	Apr	4	16:50	1997	multiflo/gem/dataall.f
r--r--r--	0/1	34519	Apr	4	16:50	1997	multiflo/gem/database.f
r--r--r--	0/1	5909	Apr	4	16:50	1997	multiflo/gem/density.f
r--r--r--	0/1	6167	Apr	4	16:50	1997	multiflo/gem/difoft.f
r--r--r--	0/1	11930	Apr	4	16:50	1997	multiflo/gem/explicit.f
r--r--r--	0/1	4443	Apr	4	16:50	1997	multiflo/gem/fkinet.f
r--r--r--	0/1	4426	Apr	4	16:50	1997	multiflo/gem/flgk.f
r--r--r--	0/1	10133	Apr	4	16:50	1997	multiflo/gem/fun.f
r--r--r--	0/1	9590	Apr	4	16:50	1997	multiflo/gem/gameq.f
r--r--r--	0/1	8730	Apr	4	16:50	1997	multiflo/gem/gamextd.f
r--r--r--	0/1	11104	Apr	4	16:50	1997	multiflo/gem/ghostpsi.f
r--r--r--	0/1	18386	Apr	4	16:50	1997	multiflo/gem/graph1d.f
r--r--r--	0/1	20775	Apr	4	16:50	1997	multiflo/gem/graph2d.f
r--r--r--	0/1	16284	Apr	4	16:50	1997	multiflo/gem/graph3d.f
r--r--r--	0/1	9298	Apr	4	16:50	1997	multiflo/gem/grid.f
r--r--r--	0/1	10441	Apr	4	16:50	1997	multiflo/gem/grid1d.f
r--r--r--	0/1	10066	Apr	4	16:50	1997	multiflo/gem/gunits.f
r--r--r--	0/1	20474	Apr	4	16:50	1997	multiflo/gem/hybrid.f
r--r--r--	0/1	37281	Apr	4	16:50	1997	multiflo/gem/initgem.f
r--r--r--	0/1	9260	Apr	4	16:50	1997	multiflo/gem/initrate.f
r--r--r--	0/1	8579	Apr	4	16:50	1997	multiflo/gem/interp.f
r--r--r--	0/1	7262	Apr	4	16:50	1997	multiflo/gem/ionexc.f
r--r--r--	0/1	9386	Apr	4	16:50	1997	multiflo/gem/kinrxn.f
r--r--r--	0/1	9623	Apr	4	16:50	1997	multiflo/gem/kinrxn_orig.f
r--r--r--	0/1	8807	Apr	4	16:50	1997	multiflo/gem/kinrxnex.f
r--r--r--	0/1	4582	Apr	4	16:50	1997	multiflo/gem/lubksb.f

5/8

19/79

```

r--r--r-- 0/1 5447 Apr 4 16:50 1997 multiflo/gem/ludcmp.f
r--r--r-- 0/1 35902 Apr 4 16:50 1997 multiflo/gem/maingem.f
r--r--r-- 0/1 6246 Apr 4 16:50 1997 multiflo/gem/massbal.f
r--r--r-- 0/1 6966 Apr 4 16:50 1997 multiflo/gem/mastrnex.f
r--r--r-- 0/1 7605 Apr 4 16:50 1997 multiflo/gem/mastrnim.f
r--r--r-- 0/1 7994 Apr 4 16:50 1997 multiflo/gem/mastrnos.f
r--r--r-- 0/1 5238 Apr 4 16:50 1997 multiflo/gem/maxchg.f
r--r--r-- 0/1 9393 Apr 4 16:50 1997 multiflo/gem/mltpsiex.f
r--r--r-- 0/1 6760 Apr 4 16:50 1997 multiflo/gem/modbnd.f
r--r--r-- 0/1 4432 Apr 4 16:50 1997 multiflo/gem/mprove.f
r--r--r-- 0/1 8448 Apr 4 16:50 1997 multiflo/gem/opspltex.f
r--r--r-- 0/1 14977 Apr 4 16:50 1997 multiflo/gem/opspltgl.f
r--r--r-- 0/1 7145 Apr 4 16:50 1997 multiflo/gem/opspltim.f
r--r--r-- 0/1 22284 Apr 4 16:50 1997 multiflo/gem/output1.f
r--r--r-- 0/1 21184 Apr 4 16:50 1997 multiflo/gem/output2.f
r--r--r-- 0/1 36959 Apr 4 16:50 1997 multiflo/gem/path.f
r--r--r-- 0/1 15082 Apr 4 16:50 1997 multiflo/gem/pecletnr.f
r--r--r-- 0/1 4844 Apr 4 16:50 1997 multiflo/gem/psat.f
r--r--r-- 0/1 61274 Apr 4 16:50 1997 multiflo/gem/readat.f
r--r--r-- 0/1 6835 Apr 4 16:50 1997 multiflo/gem/solprd.f
r--r--r-- 0/1 8906 Apr 4 16:50 1997 multiflo/gem/solprodt.f
r--r--r-- 0/1 23176 Apr 4 16:50 1997 multiflo/gem/solver.f
r--r--r-- 0/1 8573 Apr 4 16:50 1997 multiflo/gem/speciate.f
r--r--r-- 0/1 15318 Apr 4 16:50 1997 multiflo/gem/startup.f
r--r--r-- 0/1 10830 Apr 4 16:50 1997 multiflo/gem/stdyst.f
r--r--r-- 0/1 6971 Apr 4 16:50 1997 multiflo/gem/stepgem.f
r--r--r-- 0/1 12786 Apr 4 16:50 1997 multiflo/gem/testgem.f
r--r--r-- 0/1 7885 Apr 4 16:50 1997 multiflo/gem/textab.f
r--r--r-- 0/1 9534 Apr 4 16:50 1997 multiflo/gem/transp.f
rw-r--r-- 0/1 153144 Feb 28 18:16 1997 multiflo/gem/gem_qa.tar.gz
rw-r--r-- 0/11124941 Mar 6 09:16 1997 multiflo/gem/gemaster.for
rw-r--r-- 0/1 90226 Dec 19 10:26 1995 multiflo/gem/.dir.tiff
rwxr-xr-x 0/1 0 Apr 4 16:48 1997 multiflo/gem/bin/
rw-r--r-- 0/1 16556 Apr 3 11:53 1997 multiflo/gem/bin/allotgem.o
rw-r--r-- 0/1 1456 Apr 3 11:53 1997 multiflo/gem/bin/blkdtgem.o
rw-r--r-- 0/1 7320 Apr 3 11:53 1997 multiflo/gem/bin/bndcond.o
rw-r--r-- 0/1 12480 Apr 3 11:53 1997 multiflo/gem/bin/cehyliq.o
rw-r--r-- 0/1 21544 Apr 3 11:54 1997 multiflo/gem/bin/cehytwph.o
rw-r--r-- 0/1 17552 Apr 3 11:54 1997 multiflo/gem/bin/cetvdlq.o
rw-r--r-- 0/1 32304 Apr 3 11:55 1997 multiflo/gem/bin/cetvdtwp.o
rw-r--r-- 0/1 1372 Apr 3 11:53 1997 multiflo/gem/bin/cexact.o
rw-r--r-- 0/1 11704 Apr 3 11:55 1997 multiflo/gem/bin/cgasos.o
rw-r--r-- 0/1 23708 Apr 3 11:56 1997 multiflo/gem/bin/cihytwph.o
rw-r--r-- 0/1 11496 Apr 3 11:56 1997 multiflo/gem/bin/cliqos.o
rw-r--r-- 0/1 9184 Apr 3 11:53 1997 multiflo/gem/bin/coefrxn.o
rw-r--r-- 0/1 12488 Apr 3 11:56 1997 multiflo/gem/bin/coshyliq.o
rw-r--r-- 0/1 16992 Apr 3 11:56 1997 multiflo/gem/bin/dataall.o
rw-r--r-- 0/1 67872 Apr 3 11:57 1997 multiflo/gem/bin/database.o
rw-r--r-- 0/1 3524 Apr 3 11:57 1997 multiflo/gem/bin/density.o
rw-r--r-- 0/1 2840 Apr 3 11:57 1997 multiflo/gem/bin/difoft.o
rw-r--r-- 0/1 9056 Apr 3 11:57 1997 multiflo/gem/bin/eqjac.o
rw-r--r-- 0/1 18956 Apr 3 11:57 1997 multiflo/gem/bin/eqlib.o
rw-r--r-- 0/1 9040 Apr 3 11:57 1997 multiflo/gem/bin/eqres.o
rw-r--r-- 0/1 10104 Apr 3 11:58 1997 multiflo/gem/bin/explicit.o
rw-r--r-- 0/1 1160 Apr 3 11:58 1997 multiflo/gem/bin/fit.o
rw-r--r-- 0/1 1184 Apr 3 11:58 1997 multiflo/gem/bin/fkinet.o
rw-r--r-- 0/1 304 Apr 3 11:58 1997 multiflo/gem/bin/flogk.o
rw-r--r-- 0/1 16016 Apr 3 11:58 1997 multiflo/gem/bin/fun.o
rwxr-xr-x 0/11073152 Apr 3 17:56 1997 multiflo/gem/bin/gem
rw-r--r-- 0/1 7732 Apr 3 11:58 1997 multiflo/gem/bin/gameq.o

```

6/8

20/79

rw-r--r--	0/1	8688	Apr	3	11:58	1997	multiflo/gem/bin/gamextd.o
rw-r--r--	0/1	11804	Apr	3	11:58	1997	multiflo/gem/bin/ghostpsi.o
rw-r--r--	0/1	35240	Apr	3	11:58	1997	multiflo/gem/bin/graph1d.o
rw-r--r--	0/1	59180	Apr	3	11:58	1997	multiflo/gem/bin/graph2d.o
rw-r--r--	0/1	40624	Apr	3	11:59	1997	multiflo/gem/bin/graph3d.o
rw-r--r--	0/1	11644	Apr	3	11:59	1997	multiflo/gem/bin/grid.o
rw-r--r--	0/1	15928	Apr	3	11:59	1997	multiflo/gem/bin/grid1d.o
rw-r--r--	0/1	12624	Apr	3	11:59	1997	multiflo/gem/bin/gunits.o
rw-r--r--	0/1	30512	Apr	3	11:59	1997	multiflo/gem/bin/hybrid.o
rw-r--r--	0/1	90716	Apr	3	12:39	1997	multiflo/gem/bin/initgem.o
rw-r--r--	0/1	6044	Apr	3	12:00	1997	multiflo/gem/bin/initrate.o
rw-r--r--	0/1	6364	Apr	3	12:00	1997	multiflo/gem/bin/interp.o
rw-r--r--	0/1	6744	Apr	3	12:00	1997	multiflo/gem/bin/ionexc.o
rw-r--r--	0/1	8496	Apr	3	12:00	1997	multiflo/gem/bin/kinrxn.o
rw-r--r--	0/1	7656	Apr	3	12:00	1997	multiflo/gem/bin/kinrxnex.o
rw-r--r--	0/1	1032	Apr	3	12:00	1997	multiflo/gem/bin/lubksb.o
rw-r--r--	0/1	3088	Apr	3	12:00	1997	multiflo/gem/bin/ludcmp.o
rw-r--r--	0/1	42704	Apr	3	17:56	1997	multiflo/gem/bin/maingem.o
rw-r--r--	0/1	4620	Apr	3	12:01	1997	multiflo/gem/bin/massbal.o
rw-r--r--	0/1	4476	Apr	3	12:01	1997	multiflo/gem/bin/mastrnex.o
rw-r--r--	0/1	4912	Apr	3	12:01	1997	multiflo/gem/bin/mastrnim.o
rw-r--r--	0/1	5076	Apr	3	12:01	1997	multiflo/gem/bin/mastrnos.o
rw-r--r--	0/1	940	Apr	3	12:01	1997	multiflo/gem/bin/maxchg.o
rw-r--r--	0/1	9316	Apr	3	12:01	1997	multiflo/gem/bin/mltpsiex.o
rw-r--r--	0/1	4556	Apr	3	12:01	1997	multiflo/gem/bin/modbnd.o
rw-r--r--	0/1	752	Apr	3	12:01	1997	multiflo/gem/bin/mprove.o
rw-r--r--	0/1	5252	Apr	3	12:01	1997	multiflo/gem/bin/opspltex.o
rw-r--r--	0/1	14520	Apr	3	12:01	1997	multiflo/gem/bin/opspltgl.o
rw-r--r--	0/1	2980	Apr	3	12:01	1997	multiflo/gem/bin/opspltim.o
rw-r--r--	0/1	52432	Apr	3	12:01	1997	multiflo/gem/bin/output1.o
rw-r--r--	0/1	60916	Apr	3	12:01	1997	multiflo/gem/bin/output2.o
rw-r--r--	0/1	46260	Apr	3	12:02	1997	multiflo/gem/bin/path.o
rw-r--r--	0/1	17588	Apr	3	12:02	1997	multiflo/gem/bin/pecletnr.o
rw-r--r--	0/1	1652	Apr	3	12:02	1997	multiflo/gem/bin/psat.o
rw-r--r--	0/1	127412	Apr	3	17:49	1997	multiflo/gem/bin/readat.o
rw-r--r--	0/1	6016	Apr	3	12:03	1997	multiflo/gem/bin/solprd.o
rw-r--r--	0/1	12720	Apr	3	12:03	1997	multiflo/gem/bin/solprodt.o
rw-r--r--	0/1	13684	Apr	3	12:03	1997	multiflo/gem/bin/solver.o
rw-r--r--	0/1	13712	Apr	3	12:03	1997	multiflo/gem/bin/speciate.o
rw-r--r--	0/1	20984	Apr	3	17:39	1997	multiflo/gem/bin/startup.o
rw-r--r--	0/1	11500	Apr	3	12:00	1997	multiflo/gem/bin/stdyst.o
rw-r--r--	0/1	3528	Apr	3	12:04	1997	multiflo/gem/bin/stepgem.o
rw-r--r--	0/1	32064	Apr	3	12:04	1997	multiflo/gem/bin/testgem.o
rw-r--r--	0/1	18444	Apr	3	12:04	1997	multiflo/gem/bin/textab.o
rw-r--r--	0/1	7748	Apr	3	12:00	1997	multiflo/gem/bin/transp.o
rw-r--r--	0/1	4800	Apr	3	12:04	1997	multiflo/gem/bin/unitconv.o
rw-r--r--	0/1	47868	Apr	3	12:26	1997	multiflo/gem/bin/updtgem.o
rw-r--r--	0/1	55444	Apr	3	12:05	1997	multiflo/gem/bin/watsolv.o
rw-r--r--	0/1	3548	Apr	3	12:05	1997	multiflo/gem/bin/zonek.o
r--r--r--	0/1	6254	Apr	4	16:50	1997	multiflo/gem/unitconv.f
r--r--r--	0/1	24823	Apr	4	16:50	1997	multiflo/gem/updtgem.f
r--r--r--	0/1	50618	Apr	4	16:50	1997	multiflo/gem/watsolv.f
r--r--r--	0/1	1286	Apr	4	16:50	1997	multiflo/gem/addgem.h
r--r--r--	0/1	3485	Apr	4	16:50	1997	multiflo/gem/comgem.h
r--r--r--	0/1	319	Apr	4	16:50	1997	multiflo/gem/cxkin.h
r--r--r--	0/1	141	Apr	4	16:50	1997	multiflo/gem/debye.h
r--r--r--	0/1	295	Apr	4	16:50	1997	multiflo/gem/fields.h
r--r--r--	0/1	503	Apr	4	16:50	1997	multiflo/gem/frfmt.h
r--r--r--	0/1	72	Apr	4	16:50	1997	multiflo/gem/gas.h
r--r--r--	0/1	179	Apr	4	16:50	1997	multiflo/gem/impl.h

7/8

21/79

```
r--r--r-- 0/1 157 Apr 4 16:50 1997 multiflo/gem/iounits.h
r--r--r-- 0/1 337 Apr 4 16:50 1997 multiflo/gem/kinetic.h
r--r--r-- 0/1 958 Apr 4 16:50 1997 multiflo/gem/metragem.h
r--r--r-- 0/1 86 Apr 4 16:50 1997 multiflo/gem/minrl.h
r--r--r-- 0/1 516 Apr 4 16:50 1997 multiflo/gem/ofiles.h
r--r--r-- 0/1 1794 Apr 4 16:50 1997 multiflo/gem/paramtrs.h
r--r--r-- 0/1 1054 Apr 4 16:50 1997 multiflo/gem/scalgem.h
r--r--r-- 0/1 271 Apr 4 16:50 1997 multiflo/gem/scratch.h
r--r--r-- 0/1 354 Apr 4 16:50 1997 multiflo/gem/surfkin.h
r--r--r-- 0/1 68 Apr 4 16:50 1997 multiflo/gem/tempfld.h
r--r--r-- 0/1 63 Apr 4 16:50 1997 multiflo/gem/velsat.h
r--r--r-- 0/1 276 Apr 4 16:50 1997 multiflo/gem/watsolv.h
r--r--r-- 0/1 1241 Apr 4 16:50 1997 multiflo/gem/Makefile
rw-r--r-- 0/1 181 Apr 4 16:47 1997 multiflo/README
r--r--r-- 0/1 20004 Apr 4 16:12 1997 multiflo/gem.f
r--r--r-- 0/1 30033 Apr 4 16:12 1997 multiflo/mainmli.f
r--r--r-- 0/1 22801 Apr 4 16:12 1997 multiflo/metra.f
rwxr-xr-x 0/1 0 Apr 3 18:03 1997 multiflo/doc/
rwxr-xr-x 0/1 32646 Jan 28 15:05 1997 multiflo/doc/training.wp
rw-r--r-- 0/1 3034 Mar 6 14:27 1997 multiflo/doc/multi_qa.txt
rw-rw-rw- 0/1 261 Mar 26 10:48 1997 multiflo/doc/qa1.txt
rw-r--r-- 0/1 967 Mar 12 16:16 1997 multiflo/doc/listoffiles.txt
rw-r--r-- 0/1 1622 Apr 3 11:01 1997 multiflo/doc/release.txt
rw-rw-rw- 0/1 1749 Mar 26 10:48 1997 multiflo/doc/qa2.txt
rw-r--r-- 0/1 608937 Mar 27 10:16 1997 multiflo/doc/copyright.txt
rw-r--r-- 0/1 152 Apr 3 14:14 1997 multiflo/doc/sep.txt
rwxr-xr-x 0/1 158 Mar 27 10:07 1997 multiflo/doc/copyright
rw-r--r-- 0/1 465 Mar 26 15:44 1997 multiflo/doc/mod4.awk
rw-r--r-- 0/1 3966 Mar 27 10:14 1997 multiflo/doc/copylist.log
rw-r--r-- 0/1 714 Mar 26 15:34 1997 multiflo/doc/copylist.tex
rw-r--r-- 0/1 8 Mar 27 10:14 1997 multiflo/doc/copylist.aux
rw-r--r-- 0/1 684368 Mar 27 10:14 1997 multiflo/doc/copylist.dvi
rwxr-xr-x 0/1 0 Mar 27 10:24 1997 multiflo/doc/orig_metra/
rw-r--r-- 0/1 55602 Feb 19 09:32 1997 multiflo/doc/orig_metra/init.f
rw-r--r-- 0/1 18665 Mar 10 15:40 1997 multiflo/doc/orig_metra/emip.f
rw-r--r-- 0/1 27800 Feb 19 09:32 1997 multiflo/doc/orig_metra/outmetra.f
rw-r--r-- 0/1 13825 Feb 19 09:32 1997 multiflo/doc/orig_metra/openfls.f
rw-r--r-- 0/1 52884 Mar 5 09:42 1997 multiflo/doc/orig_metra/recdat.f
rw-r--r-- 0/1 18338 Feb 19 09:32 1997 multiflo/doc/orig_metra/emip.0
rw-r--r-- 0/1 5760 Apr 3 13:51 1997 multiflo/doc/tree_gem.txt
rw-r--r-- 0/1 4606 Apr 3 16:32 1997 multiflo/doc/tree_metra.txt
rwxr-xr-x 0/1 0 Apr 4 16:45 1997 multiflo/SCCS/
r--r--r-- 0/1 20352 Apr 4 16:45 1997 multiflo/SCCS/s.gem.f
r--r--r-- 0/1 30381 Apr 4 16:45 1997 multiflo/SCCS/s.mainmli.f
r--r--r-- 0/1 23149 Apr 4 16:45 1997 multiflo/SCCS/s.metra.f
r--r--r-- 0/1 461 Apr 4 16:45 1997 multiflo/SCCS/s.misc.f
r--r--r-- 0/1 3758 Apr 4 16:45 1997 multiflo/SCCS/s.Makefile
rw-r--r-- 0/1 74225 Mar 27 10:03 1997 multiflo/multimas.for
rw-r--r-- 0/1 90226 Dec 19 10:26 1995 multiflo/.dir.tiff
rw-r--r-- 0/1 855471 Mar 27 10:03 1997 multiflo/metramas.for
rw-r--r-- 0/11030742 Mar 27 10:03 1997 multiflo/gemmas.for
rw-r--r-- 0/11960438 Mar 27 10:03 1997 multiflo/mflomas.for
rwxr-xr-x 0/1 2130 Mar 27 10:04 1997 multiflo/cat_multi
rwxr-xr-x 0/1 0 Apr 4 16:10 1997 multiflo/bin/
rwxr-xr-x 0/1 0 Apr 4 15:59 1997 multiflo/bin/database/
rw-r--r-- 0/1 123406 Apr 4 15:59 1997 multiflo/bin/database/ms25.r16
rw-r--r-- 0/1 213388 Apr 4 15:59 1997 multiflo/bin/database/mstemp.r16
rwxr-xr-x 0/11884160 Apr 3 17:47 1997 multiflo/bin/multiflo
r--r--r-- 0/1 113 Apr 4 16:12 1997 multiflo/misc.f
r--r--r-- 0/1 3410 Apr 4 16:12 1997 multiflo/Makefile
```

8/8

# CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

22/79

## DESIGN VERIFICATION REPORT FOR CNWRA SOFTWARE: MULTIFLO V. 1.0

---

April 4, 1997

### SECTION 1 - METRA

1. Scientific Notebook Documentation Development: CNWRA Electronic Scientific Notebook number 095 was verified; it is submitted quarterly, reviewed by EM, and documents the software development.
2. Programming Language: ANSI Standard FORTRAN 77 confirmed by the Software Custodian.
3. Internal Documentation: On 3/28/97, B. Mabrito reviewed portions of the METRA software on one of the CNWRA platforms. MAINMETRA.f (frfmt) and (pvth2o.f) were reviewed and there were clear and numerous internal documentation comments meeting the requirements of TOP-018 Section 5.4.4.
4. Software Labels and Data
  - a. Header Data and Format: METRA header data and the format were compared against TOP-018 Section 5.4.6 and found acceptable (file MAINMETRA.f). See attached sheets.
  - b. NRC Data: METRA header data and the format were compared against TOP-018, Section 5.4.6, fourth bullet and found acceptable.
  - c. Source Code Header: METRA header data was compared to TOP-018 Section 5.4.6, fifth bullet, and found acceptable.
5. Unique Run Identification: At the top of each output file a unique identifier was created on the print out. For instance, a page of the file printed and attached to this report showed the following: "This file was created on: Fri Mar 28 17:04:43 1997" which fully meets the unique run identification requirements.
6. Software Analysis and Results
  - a. Analysis: FOR\_STUDY Version 1.2 was utilized as the software analysis tool. FOR\_STUDY was run in the "default configuration" as specified in the Users Manual and this was the first use at the CNWRA of the FOR\_STUDY analysis tool.
  - b. Analysis Report: Portions of the analysis report have been printed and several pages have been attached to this document. The analysis report electronic file was provided to the METRA software developer and he utilized it to identify areas of concern and a bug which he had been trying to locate. A total of 555 warning messages from FOR\_STUDY were listed and the developer reviewed them all.

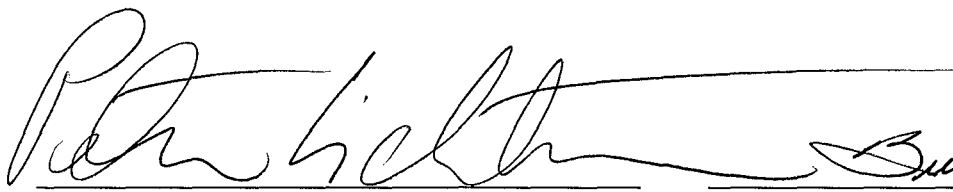
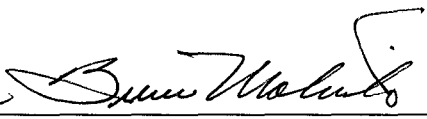
c. Resolution of Comments: The developer reviewed all of the warning and error messages and addressed the most critical problem statements. According to the developer, only one serious error to the module existed and was discovered by the FOR\_STUDY software analysis tool. That was in the call to slvliq.f in METRA in which the final argument aa was missing. The software developer is knowledgeable of the current warnings and errors and accepts them.

## Section 2 - GEM

1. Scientific Notebook Documentation Development: CNWRA Electronic Scientific Notebook number 095 was verified; the Scientific Notebook is submitted quarterly and it documents the software development.
2. Programming Language: ANSI Standard FORTRAN 77 was confirmed by the Software Custodian.
3. Internal Documentation: On 4/3/97, B. Mabrito reviewed portions of the GEM software on one of the CNWRA platforms. MAINGEM.f was reviewed and it was confirmed that there is clear and numerous internal documentation comments meeting the requirements of TOP-018 Section 5.4.4.
4. Software Labels and Data:
  - a. Header Data and Format: GEM header data and the format were compared against TOP-018 Section 5.4.6 and found acceptable. See attached sheets.
  - b. NRC Data: GEM header data and the format were compared against TOP-018, Section 5.4.6, fourth bullet and found acceptable.
  - c. Source Code Header: GEM header data was compared to TOP-018 Section 5.4.6, fifth bullet, and found acceptable.
5. Unique Run Identification: At the top of each output file a unique identifier states for each print out the following: "This file was created on: xxx xxx x xx:xx:xx." This identifier meets the requirements of unique run identification.
6. Software Analysis and Results
  - a. Analysis: Software analysis tool FOR\_STUDY Version 1.2 was utilized on GEM. FOR\_STUDY was run in the "default configuration" as specified in its Users Manual. The software analysis tool was run on GEM on 4/2/97.
  - b. Analysis Report: A total of 3,802 warning messages were initially received from the FOR\_STUDY software analysis, but that number was quickly reduced to 3,403 warnings on a second run because of changes introduced by the developer. In the second FOR\_STUDY run, 5 semantic errors and zero syntax errors remained, along with the 3,403 warnings which are considered harmless by the developer.

c. Resolution of Comments: In addition to "cosmetic" changes performed by the GEM software developer to address some of the software tool warnings, one potentially serious error was found in the call to subroutine Indcond.f from cgasos.f. However, this portion of the code is not part of the current release and has not been fully tested. The software developer is knowledgeable of the current warnings and errors and accepts them.

7. MULTIFLO EXECUTIVE: There were no serious errors found in the MULTIFLO EXECUTIVE program according to the software developer.

	
<hr/>	<hr/>
CNWRA Software Developer	CNWRA Software Custodian

Attachments/

original to: Software Folder  
cc: CNWRA Software Developer

25/79

pcl4

JOB 859

pat.metra.rpt

*Analysis Results from  
FOR STUDY for METRA.  
"Warning" and "Error" STATE-  
MENTS made. Examples  
Listed. Q2 4/3/97*

For: root  
Date: Thu Apr 3 10:09:12 CST 1997  
Submit queue: Ethernet  
Submitted: 528:39:43  
Started: 528:39:43



QMS 1725 Print System

QMS 1725 (1st floor)



Warning #12 accm.f,477: common /COMBC/ was not used in function ACCM()  
Warning #72 accm.f,477: common /CHRS/ was not used in function ACCM()  
Warning #72 accm.f,477: common /PVTTAB/ was not used in function ACCM()  
Warning #9 accm.f,477: include file 'pvttbl.h' was not used in routine ACCM()  
Warning #12 accmvp.f,479: common /COMBC/ was not used in function ACCMVP()  
Warning #72 accmvp.f,479: common /CHRS/ was not used in function ACCMVP()  
Warning #72 accmvp.f,479: common /PVTTAB/ was not used in function ACCMVP()  
Warning #9 accmvp.f,479: include file 'pvttbl.h' was not used in routine ACCMVP()  
Warning #717 allot.f,330: expecting multi-dimension array - array element passed in arg #1 of ORDER()  
Warning #336 allot.f,330: different type and size used in arg #1 of ORDER()  
Warning #686 allot.f,330: different type and size used in arg #2 of ORDER()  
Warning #686 allot.f,330: different type and size used in arg #3 of ORDER()  
Warning #686 allot.f,330: different type and size used in arg #4 of ORDER()  
Warning #686 allot.f,330: different type and size used in arg #5 of ORDER()  
Warning #686 allot.f,331: different type and size used in arg #6 of ORDER()  
Warning #717 allot.f,387: expecting multi-dimension array - array element passed in arg #1 of SYMFAC()  
Warning #686 allot.f,387: different type and size used in arg #1 of SYMFAC()  
Warning #686 allot.f,387: different type and size used in arg #2 of SYMFAC()  
Warning #686 allot.f,387: different type and size used in arg #3 of SYMFAC()  
Warning #686 allot.f,387: different type and size used in arg #4 of SYMFAC()  
Warning #686 allot.f,387: different type and size used in arg #5 of SYMFAC()  
Warning #717 allot.f,388: expecting multi-dimension array - array element passed in arg #6 of SYMFAC()  
Warning #686 allot.f,388: different type and size used in arg #6 of SYMFAC()  
Warning #686 allot.f,388: different type and size used in arg #7 of SYMFAC()  
Warning #686 allot.f,388: different type and size used in arg #8 of SYMFAC()  
Warning #717 allot.f,388: expecting multi-dimension array - array element passed in arg #9 of SYMFAC()  
Warning #686 allot.f,388: different type and size used in arg #9 of SYMFAC()  
Warning #686 allot.f,388: different type and size used in arg #10 of SYMFAC()  
Warning #72 allot.f,470: common /COM1/ was not used in function ALLOT()  
Warning #72 allot.f,470: common /COM2/ was not used in function ALLOT()  
Warning #72 allot.f,470: common /COMBC/ was not used in function ALLOT()  
Warning #72 allot.f,470: common /REALS/ was not used in function ALLOT()  
Warning #72 allot.f,470: common /CHRS/ was not used in function ALLOT()  
Warning #9 allot.f,470: include file 'com.h' was not used in routine ALLOT()  
Warning #72 bcond.f,834: common /CHRS/ was not used in function BCOND()  
Warning #72 blkdtmet.f,234: common /REALNUM/ was not used in function METBLK()  
Warning #72 blkdtmet.f,234: common /CHRS/ was not used in function METBLK()  
Warning #72 blkdtmet.f,234: common /FRMT/ was not used in function METBLK()  
Warning #9 blkdtmet.f,234: include file 'impl.h' was not used in routine METBLK()  
Warning #9 blkdtmet.f,234: include file 'frfmt.h' was not used in routine METBLK()  
Warning #72 coefs.f,961: common /COMBC/ was not used in function COEFS()  
Warning #72 coefs.f,961: common /CHRS/ was not used in function COEFS()  
Warning #72 coefsvp.f,988: common /COMBC/ was not used in function COEFSVP()  
Warning #72 coefsvp.f,988: common /CHRS/ was not used in function COEFSVP()  
Warning #715 cond.f,283: expecting 2-dimension array - 1-dimension array passed in arg #2 of CCOEFS()  
Warning #715 cond.f,284: expecting 2-dimension array - 1-dimension array passed in arg #2 of CCOEFS()  
Warning #715 cond.f,285: expecting 2-dimension array - 1-dimension array passed in arg #2 of CCOEFS()  
Warning #715 cond.f,368: expecting 2-dimension array - 1-dimension array passed in arg #3 of QCOND()  
Warning #715 cond.f,368: expecting 2-dimension array - 1-dimension array passed in arg #4 of QCOND()  
Warning #715 cond.f,368: expecting 2-dimension array - 1-dimension array passed in arg #5 of QCOND()  
Warning #715 cond.f,418: expecting 2-dimension array - 1-dimension array passed in arg #1 of SOLVE()  
Warning #712 cond.f,418: expecting scalar argument - not entire array in arg #3 of SOLVE()  
Warning #712 cond.f,418: expecting scalar argument - not entire array in arg #4 of SOLVE()  
Warning #712 cond.f,418: expecting scalar argument - not entire array in arg #5 of SOLVE()  
Warning #712 cond.f,418: expecting scalar argument - not entire array in arg #6 of SOLVE()  
Warning #712 cond.f,418: expecting scalar argument - not entire array in arg #7 of SOLVE()  
Warning #712 cond.f,418: expecting scalar argument - not entire array in arg #8 of SOLVE()  
Warning #715 cond.f,459: expecting 2-dimension array - 1-dimension array passed in arg #1 of IMPFLX()  
Warning #715 cond.f,459: expecting 2-dimension array - 1-dimension array passed in arg #2 of IMPFLX()  
Warning #715 cond.f,459: expecting 2-dimension array - 1-dimension array passed in arg #3 of IMPFLX()

27/79

Warning #72 cond.f,581: common /COM2/ was not used in function COND()  
Warning #72 cond.f,581: common /CHRS/ was not used in function COND()  
Warning #72 cond.f,581: common /ADDRESS/ was not used in function COND()  
Warning #9 cond.f,581: include file 'add.h' was not used in routine COND()  
Warning #72 cond.f,796: common /COM2/ was not used in function IMPFLX()  
Warning #72 cond.f,796: common /CHRS/ was not used in function IMPFLX()  
Warning #72 cond.f,796: common /DEVICES/ was not used in function IMPFLX()  
Warning #9 cond.f,796: include file 'units.h' was not used in routine IMPFLX()  
Warning #72 cond.f,974: common /COM2/ was not used in function CCOEFS()  
Warning #72 cond.f,974: common /COMBC/ was not used in function CCOEFS()  
Warning #72 cond.f,974: common /REALS/ was not used in function CCOEFS()  
Warning #72 cond.f,974: common /INTEGRS/ was not used in function CCOEFS()  
Warning #72 cond.f,974: common /CHRS/ was not used in function CCOEFS()  
Warning #72 cond.f,974: common /DEVICES/ was not used in function CCOEFS()  
Warning #72 cond.f,974: common /ADDRESS/ was not used in function CCOEFS()  
Warning #9 cond.f,974: include file 'scalars.h' was not used in routine CCOEFS()  
Warning #9 cond.f,974: include file 'units.h' was not used in routine CCOEFS()  
Warning #72 cond.f,974: include file 'add.h' was not used in routine CCOEFS()  
Warning #72 cond.f,1192: common /COM2/ was not used in function QCOND()  
Warning #72 cond.f,1192: common /CHRS/ was not used in function QCOND()  
Warning #72 cond.f,1192: common /DEVICES/ was not used in function QCOND()  
Warning #9 cond.f,1192: include file 'units.h' was not used in routine QCOND()  
Warning #543 d4gaus.f,825: loss of precision in assignment: REAL\*4 to INTEGER\*4  
Warning #543 d4gaus.f,831: loss of precision in assignment: REAL\*4 to INTEGER\*4  
Warning #72 debug.f,215: common /REALNUM/ was not used in function DEBUG()  
Warning #9 debug.f,215: include file 'impl.h' was not used in routine DEBUG()  
Warning #72 dtstep.f,394: common /CHRS/ was not used in function AUTODT()  
Warning #72 dtstep.f,394: common /DEVICES/ was not used in function AUTODT()  
Warning #9 dtstep.f,394: include file 'units.h' was not used in routine AUTODT()  
Warning #72 dtstep.f,545: common /COM2/ was not used in function AUTOSTEP()  
Warning #72 dtstep.f,545: common /COMBC/ was not used in function AUTOSTEP()  
Warning #72 dtstep.f,545: common /INTEGRS/ was not used in function AUTOSTEP()  
Warning #72 dtstep.f,545: common /CHRS/ was not used in function AUTOSTEP()  
Warning #72 dtstep.f,575: common /REALNUM/ was not used in function DXDT()  
Warning #72 dtstep.f,575: common /REALS/ was not used in function DXDT()  
Warning #72 dtstep.f,575: common /INTEGRS/ was not used in function DXDT()  
Warning #72 dtstep.f,575: common /CHRS/ was not used in function DXDT()  
Warning #9 dtstep.f,575: include file 'impl.h' was not used in routine DXDT()  
Warning #9 dtstep.f,575: include file 'scalars.h' was not used in routine DXDT()  
Warning #72 equil.f,536: common /COMBC/ was not used in function EQUIL()  
Warning #72 equil.f,536: common /CHRS/ was not used in function EQUIL()  
Warning #543 equil.f,552: loss of precision in assignment: REAL\*8 to INTEGER\*4  
Warning #72 equil.f,577: common /INTEGRS/ was not used in function DEN()  
Warning #72 equil.f,577: common /CHRS/ was not used in function DEN()  
Warning #72 equil.f,577: common /DEVICES/ was not used in function DEN()  
Warning #9 equil.f,577: include file 'paramtrs.h' was not used in routine DEN()  
Warning #9 equil.f,577: include file 'units.h' was not used in routine DEN()  
Warning #72 griddat.f,402: common /REALNUM/ was not used in function GRIDDAT()  
Warning #72 griddat.f,402: common /COM2/ was not used in function GRIDDAT()  
Warning #72 griddat.f,402: common /COMBC/ was not used in function GRIDDAT()  
Warning #72 griddat.f,402: common /REALS/ was not used in function GRIDDAT()  
Warning #72 griddat.f,402: common /INTEGRS/ was not used in function GRIDDAT()  
Warning #72 griddat.f,402: common /CHRS/ was not used in function GRIDDAT()  
Warning #9 griddat.f,402: include file 'impl.h' was not used in routine GRIDDAT()  
Warning #9 griddat.f,402: include file 'scalars.h' was not used in routine GRIDDAT()  
Warning #72 init.f,422: expecting multi-dimension array - array element passed in arg #1 of PRINTS()  
Warning #717 init.f,422: expecting multi-dimension array - array element passed in arg #2 of PRINTS()  
Warning #713 init.f,422: expecting lvalue as scalar argument - constant/expr passed in arg #8 of PRINTS()  
Warning #715 init.f,425: expecting 3-dimension array - 1-dimension array passed in arg #1 of PRINTS()  
Warning #717 init.f,425: expecting multi-dimension array - array element passed in arg #2 of PRINTS()

Warning #713 init.f,425: expecting lvalue as scalar argument - constant/expr passed in arg #8 of PRINTS()  
Warning #715 init.f,428: expecting 3-dimension array - 1-dimension array passed in arg #1 of PRINTS()  
Warning #717 init.f,428: expecting multi-dimension array - array element passed in arg #2 of PRINTS()  
Warning #713 init.f,428: expecting lvalue as scalar argument - constant/expr passed in arg #8 of PRINTS()  
Warning #715 init.f,431: expecting 3-dimension array - 1-dimension array passed in arg #1 of PRINTS()  
Warning #717 init.f,431: expecting multi-dimension array - array element passed in arg #2 of PRINTS()  
Warning #713 init.f,431: expecting lvalue as scalar argument - constant/expr passed in arg #8 of PRINTS()  
Error #725 init.f,524: expecting FUNCTION address - not scalar (lvalue) in arg #3 of GENPVT()  
Warning #606 init.f,524: different type and size used in arg #3 of GENPVT()  
Warning #513 init.f,660: loss of precision in assignment: REAL\*8 to INTEGER\*4  
Warning #543 init.f,726: loss of precision in assignment: REAL\*8 to INTEGER\*4  
Warning #713 init.f,734: expecting lvalue as scalar argument - constant/expr passed in arg #19 of PCKR()  
Warning #713 init.f,743: expecting lvalue as scalar argument - constant/expr passed in arg #2 of PVT()  
Error #725 init.f,743: expecting FUNCTION address - not scalar (lvalue) in arg #3 of PVT()  
Warning #606 init.f,743: different type and size used in arg #3 of PVT()  
Warning #713 init.f,778: expecting lvalue as scalar argument - constant/expr passed in arg #2 of PVTVP()  
Error #725 init.f,778: expecting FUNCTION address - not scalar (lvalue) in arg #3 of PVTVP()  
Warning #606 init.f,778: different type and size used in arg #3 of PVTVP()  
Warning #713 init.f,1574: common /COM2/ was not used in function INIT1()  
Warning #713 init.f,1574: common /COMBC/ was not used in function INIT1()  
Warning #713 init.f,1574: common /CHRS/ was not used in function INIT1()  
Warning #713 init.f,1823: common /CHRS/ was not used in function GENPVT()  
Warning #713 init.f,1823: include file 'paramtrs.h' was not used in routine GENPVT()  
Warning #314 inpmetra.f,380: mixed strings and arithmetic objects in arg #2 of XOPEN()  
Warning #543 inpmetra.f,603: loss of precision in assignment: REAL\*8 to INTEGER\*4  
Warning #543 inpmetra.f,687: mixed strings and arithmetic objects in arg #2 of XOPEN()  
Warning #543 inpmetra.f,783: mixed strings and arithmetic objects in arg #2 of XOPEN()  
Warning #543 inpmetra.f,876: loss of precision in assignment: REAL\*8 to INTEGER\*4  
Warning #543 inpmetra.f,954: loss of precision in assignment: REAL\*8 to INTEGER\*4  
Warning #543 inpmetra.f,977: loss of precision in assignment: REAL\*8 to INTEGER\*4

29/79

**postscript**

**JOB 665**

**UNTITLED -- /u01/lichtner\_u01/metra**

**For:** lichtner  
**Date:** Fri Mar 28 18:14:00 CST 1997  
**Creator:** Edit  
**Creation Date:** Fri Mar 28 18:10:04 1997  
  
**Submit queue:** Ethernet  
**Submitted:** 396:24:10  
**Started:** 396:24:11



**QMS 1725 Print System**

**QMS 1725 (1st floor)**

30/79

-----  
FOR\_STUDY v2.0.1 LOCAL REPORTS - Created on 03/27/1997 at 14:16:07  
-----

FOR\_STUDY Options SET:

FOR=sun FX=a&befiklmnqstuxz" FXS=ap FXV=adorv% GREPT=cdefnTu REP=aImnSUX S=aiz  
V=fo W=acdefilnopqstuwyr%

\*\*\*\*\* FUNCTION INTERFACE \*\*\*\*\*

```

SUBROUTINE ACCM(c,r)
  REAL*8,          INTENT(INOUT)::c(3,3,*)
  REAL*8,          INTENT(INOUT)::r(3,*)
*   Location:  accm.f,207-477
*   Commons:   /REALNUM/:R /METGEM/:R /COM1/:R /COM2/:R /REALS/:R
*             /INTEGRS/:R /DEVICES/:R
*   I/O Units: IFBUG[W]
END SUBROUTINE

```

\*\*\*\*\*

Location Key:

a(decl'd) T(typed) t(implicitly typed) =(set) e=(set via equiv)  
e(referenced via equiv) or simply ref'd at the line number

ARGUMENT REFERENCES FOR SUBROUTINE ACCM()

Name	Class	Type	Location(s) in accm.f							
-----										
c(3,*,*)	! set diagonal coefs to a large number									
	ARRAY	dblp	218d	305t=	306=	307=	311=	312=		
			313=	317=	318=	319=	365=	366=		
			367=	374=	375=	376=	387=	388=		
			389=	418=	419=	420=	425=	426=		
			427=	431=	432=	433=	442=	448=		
			450=	466	467	468				
r(3,*)	ARRAY	dblp	218d	292t=	293=	294=	337=	338=		
			339=	403=	404=	405=	443=	451=		
			466	467	468					

CROSS REFERENCE FOR SUBROUTINE ACCM() - Primary File Only

Name	Class	Type	Location(s) in accm.f							
-----										
AG	VAR	dblp	360t=	365	374	387	410=	418		
			425	431						
BN	VAR	dblp	299t=	305	311	317	352=	365		
			374	387						
BG	VAR	dblp	359t=	366	375	388	411=	419		
			426	432						
BW	VAR	dblp	351t=	366	375	388				

-----  
 FOR\_STUDY v2.0.1 GLOBAL REPORTS - Created on 03/27/1997 at 14:16:07  
 -----

FOR\_STUDY Options SET:

FOR=sun FX=a&befiklmngstuxz" FXS=ap FXV=adorv% GREPT=cdefnTu REP=aImnSUX S=aiz  
 V=fo W=acdefilnopqstuwyr%

FUNCTION SUMMARY

Class Name	Location	Calls	Call Sites
SUBR ACCM()	accm.f,207	0 !!!	
SUBR ACCMVP()	accmvp.f,207	0 !!!	
SUBR ALLOT()	allot.f,195	3	MAIN00() RECDAT()
SUBR AUTODT()	dtstep.f,179	1	MAIN00()
SUBR AUTOSTEP()	dtstep.f,395	2	MAIN00()
SUBR BCOND()	bcond.f,258	3	SOURCE()
SUBR BINTERP()	trans.f,473	3	TRANS()
SUBR CCOEFS()	cond.f,797	3	COND()
SUBR CGSTAB()	watsolv.f,577	1	WATSOLV()
SUBR CHECK_UPDATE()	watsolv.f,905	2	CGSTAB() GMRES()
SUBR CMDLIN()	openfls.f,513	1	OPENFLS()
SUBR COEFS()	coefs.f,265	0 !!!	
SUBR COEFSVP()	coefsvp.f,265	0 !!!	
SUBR COND()	cond.f,244	1	MAIN00()
SUBR CONVERT()	mainmetra.f,919	10	GRIDDAT() INPMETRA() MAIN00() FRFMT() RECDAT() INPBC()
SUBR CPUTIM()	mainmetra.f,1043	25	COND() ITER() MAIN00() SLVLIQ()
FUNCTION CPUTIME()	watsolv.f,550	2	WATSOLV()
SUBR D4GAUS()	d4gaus.f,237	2	SOLVE()
SUBR DAXPY()	watsolv.f,1146	4	GMRES()
SUBR DCOPY()	watsolv.f,1115	2	WATSOLV() GMRES()
FUNCTION DDOT()	watsolv.f,1130	5	CGSTAB() GMRES()
SUBR DEBUG()	debug.f,158	1	SOLVE()
FUNCTION DEN()	equil.f,537	3	EQUIL()
FUNCTION DNRM2()	watsolv.f,1198	2	WATSOLV() GMRES()
SUBR DSCAL()	watsolv.f,1163	2	GMRES()
FUNCTION DTIME()	misc.f,6	0 !!!	
SUBR DXDT()	dtstep.f,546	3	AUTOSTEP()
SUBR ECMTBL1()	ecmtbl.f,202	1	INIT()
SUBR ECMTBL2()	ecmtbl.f,476	1	INIT()
SUBR EMIP()	emip.f,249	2	INIT() OUTMETRA()
SUBR EQUIL()	equil.f,208	1	INIT()
FUNCTION ETIME()	-	1	SECONDS()
SUBR FACTOR()	watsolv.f,1008	1	WATSOLV()
SUBR FDATE()	misc.f,1	0 !!!	
SUBR FLUXES()	outmetra.f,748	3	OUTMETRA()
SUBR FRFMT()	mainmetra.f,719	22	GRIDDAT() INPMETRA() READ() MAIN00() RECDAT() INPBC() INPSRC()
SUBR GENPVT()	init.f,1575	1	INIT()
FUNCTION GETARG()	-	1	CMDLIN()
SUBR GETFIL()	openfls.f,310	6	OPENFLS()
SUBR GMRES()	watsolv.f,709	1	WATSOLV()
SUBR GRIDDAT()	griddat.f,223	1	INPMETRA()
BLOCK H2O()		0	
FUNCTION IDAMAX()	watsolv.f,1178	3	WATSOLV() GMRES()
SUBR IMPFLX()	cond.f,582	1	COND()
SUBR INIT()	init.f,308	1	MAIN00()
SUBR INIT1()	init.f,1111	1	INIT()

SUBR	INPBC()	recdat.f,930	1	RECDAT()	
SUBR	INPMETRA()	inpmetra.f,191	1	MAIN00()	
SUBR	INPSRC()	recdat.f,1316	1	RECDAT()	
SUBR	ITER()	iter.f,262	2	MAIN00()	
FUNCTION	LENSYM()	openfls.f,419	14	OPENFLS()	PLOTS()
FUNCTION	LNBLNK()	mainmetra.f,1176	5	CMDLIN()	OPENFILE()
SUBR	LUSOLV()	watsolv.f,931	5	WATSOLV()	CGSTAB()
				GMRES()	
FUNCTION	MAIN00()		1		
BLOCK	METBLK()		0		
BLOCK	METRAGEM()		0		
SUBR	MVMULT()	watsolv.f,972	5	WATSOLV()	CGSTAB()
				GMRES()	
SUBR	OPENFILE()	plots.f,1003	18	PLOTS()	
SUBR	OPENFLS()	openfls.f,133	5	EMIP()	INPMETRA()
				MAIN00()	RECDAT()
SUBR	ORDER()	d4gaus.f,686	1	ALLOT()	
SUBR	OUTMETRA()	outmetra.f,244	1	MAIN00()	
SUBR	PCKR()	pckr.f,209	4	INIT()	ITER()
				SETBC()	
FUNCTION	PCW()	pvtfunc.f,519	2	EQUIL()	PVTVP()
SUBR	PLOTS()	plots.f,157	1	OUTMETRA()	
SUBR	PRINTS()	prints.f,139	18	INIT()	INPMETRA()
				OUTMETRA()	
FUNCTION	PSK()	pvtfunc.f,159	10	GENPVT()	UPDTPSK()
				UPDTVPK()	
SUBR	PVT()	pvt.f,172	1	INIT()	
SUBR	PVTH20()	pvth2o.f,167	0	!!!	
SUBR	PVTVP()	pvtvp.f,182	1	INIT()	
SUBR	QCOND()	cond.f,975	1	COND()	
FUNCTION	RAND()	-	1	RANDF()	
FUNCTION	RANFD()	inpmetra.f,1540	2	RANFLD()	
SUBR	RANFLD()	inpmetra.f,1425	1	INPMETRA()	
SUBR	RANGE()	inpmetra.f,1306	6	INPMETRA()	RECDAT()
				INPBC()	INPSRC()
FUNCTION	READ()	inpmetra.f,1190	3	INPMETRA()	
SUBR	RECDAT()	recdat.f,192	1	MAIN00()	
FUNCTION	RND()	inpmetra.f,1558	0	!!!	
SUBR	RSTART()	rstart.f,165	2	MAIN00()	OUTMETRA()
SUBR	SECONDS()	mainmetra.f,1130	3	CPUTIM()	CPUTIME()
SUBR	SETBC()	setbc.f,177	1	MAIN00()	
SUBR	SLVLIQ()	slvliq.f,266	1	MAIN00()	
SUBR	SOLVE()	solve.f,210	3	COND()	ITER()
				SLVLIQ()	
SUBR	SOURCE()	source.f,202	2	ITER()	SLVLIQ()
SUBR	SYMFAC()	watsolv.f,1325	1	ALLOT()	
SUBR	THOMAS1()	thomas.f,152	4	SOLVE()	
SUBR	THOMAS3()	thomas.f,279	4	SOLVE()	
FUNCTION	TKVP()	pvtfunc.f,224	1	PVTVP()	
SUBR	TRANS()	trans.f,194	3	INIT()	ITER()
				SLVLIQ()	
FUNCTION	TS()	pvtfunc.f,418	3	PVT()	UPDTPSK()
				UPDTVPK()	
SUBR	UPDATE()	update.f,170	1	MAIN00()	
SUBR	UPDTPSK()	updtpsk.f,248	0	!!!	
SUBR	UPDTVPK()	updtvpk.f,251	0	!!!	
SUBR	VISGAS()	pckr.f,702	1	PCKR()	
SUBR	VISH20()	pvth2o.f,596	0	!!!	
SUBR	WATSOLV()	watsolv.f,242	2	SOLVE()	
SUBR	XOPEN()	recdat.f,1676	5	INPMETRA()	INPBC()
				INPSRC()	

# Summary 79 Functions Defined and Called

11 Functions Defined, but not Called  
 3 Functions Called, but not Defined  
 0 Library routines Called

3 Block Data routines

----

96 Total Function References and Definitions



FOR-STUDY 34/79  
PRINT OUT  
example.

Warning #626 slvliq.f,293: differing number of TRANS() arguments; intrf.  
vs. call

Warning #715 slvliq.f,379: expecting 3-dimension array - 1-dimension  
array passed in arg #1 of SOURCE()

Warning #715 slvliq.f,379: expecting 2-dimension array - 1-dimension  
array passed in arg #2 of SOURCE()

Warning #715 slvliq.f,379: expecting 2-dimension array - 1-dimension  
array passed in arg #3 of SOURCE()

Warning #715 slvliq.f,379: expecting 2-dimension array - 1-dimension  
array passed in arg #4 of SOURCE()

Warning #715 slvliq.f,379: expecting 2-dimension array - 1-dimension  
array passed in arg #5 of SOURCE()

Warning #715 slvliq.f,379: expecting 1-dimension array - 3-dimension  
array passed in arg #6 of SOURCE()

Warning #715 slvliq.f,379: expecting 1-dimension array - 3-dimension  
array passed in arg #7 of SOURCE()

Warning #715 slvliq.f,379: expecting 1-dimension array - 3-dimension  
array passed in arg #8 of SOURCE()

Warning #715 slvliq.f,426: expecting 2-dimension array - 1-dimension  
array passed in arg #1 of SOLVE()

Warning #712 slvliq.f,426: expecting scalar argument - not entire array  
in arg #3 of SOLVE()

Warning #712 slvliq.f,426: expecting scalar argument - not entire array  
in arg #4 of SOLVE()

Warning #712 slvliq.f,426: expecting scalar argument - not entire array  
in arg #5 of SOLVE()

Warning #712 slvliq.f,426: expecting scalar argument - not entire array  
in arg #6 of SOLVE()

Warning #712 slvliq.f,426: expecting scalar argument - not entire array  
in arg #7 of SOLVE()

Warning #712 slvliq.f,426: expecting scalar argument - not entire array  
in arg #8 of SOLVE()

Warning #72 slvliq.f,594: common /COM2/ was not used in function  
SLVLIQ()

Warning #72 slvliq.f,594: common /CHRS/ was not used in function  
SLVLIQ()

**postscript**

**JOB 664**

**UNTITLED -- /u01/lichtner\_u01/metra**

**For:** lichtner  
**Date:** Fri Mar 28 18:13:03 CST 1997  
**Creator:** Edit  
**Creation Date:** Fri Mar 28 18:07:19 1997

**Submit queue:** Ethernet  
**Submitted:** 396:23:58  
**Started:** 396:23:59



**QMS 1725 Print System**

**QMS 1725 (1st floor)**

```
c*file mainmetra.f
```

```
c Program Name: MULTIFLO/METRA
c File/Subroutine Names: mainmetra.f/mainmetra.f frfmt.f cputim.f
c second.f
c Release Date: February, 1997
c Release Version: 1.0
c Client Name: USNRC
c Client Contact: Bret Leslie (301-415-6652)
c Contract Number: NRC 02-93-005
c CNWRA Contact: Peter C. Lichtner (210-522-6084)
c Center for Nuclear Waste Regulatory Analyses
c San Antonio, Texas 78238-5166
c lichtner@swri.edu
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

### C VERSION/REVISION HISTORY

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

Date	Author(s)	Comments/Modifications
February 97	Mohan S. Seth Peter C. Lichtner	Initial Implementation

[illegible]

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 c c c

C PURPOSE:

```
c   This is main driver program for the entire code. Essentially
c   no computations are performed by this module, but it controls
c   the flow of computations.
```

```
c      This module is replaced my metra.f when run in coupled mode with
c      multiflo.
```

[illegible]

C PROGRAMMING LANGUAGE

ANSI Standard Fortran - 77

[illegible]

This file was created on: Fri Mar 28 17:04:43 1997

Prepared for the U.S. NRC

<<< VERSION 1.0 >>>

Enhanced Memory Version: September 9, 1996

MULTICOMPONENT CHEMICAL TRANSPORT MODEL

Copyright (c) 1977 Southwest Research Institute  
All Rights Reserved

quartz dissolution  
Testing with free format and dynamic memory

QUAD--->

Co-ordinate Geometry : XYZ

Number of Elements in I-direction.....	NX =	1
Number of Elements in J-direction.....	NY =	1
Number of Elements in K-direction.....	NZ =	100
Total Number of Elements.....	NB =	100
Index for Mode of Operation .....	MODE =	2
Index for Amount of Output .....	IPRINT =	1
Index for Debugging .....	IDEBUG =	0

39/79

pcl4

JOB 860

pat.gem.rpt

*Analysis Results from  
FOR-STUDY for  
GEM. "Warning" and  
"Error" statements listed.  
Examples listed.*

*GEW 4/3/97*

For: root  
Date: Thu Apr 3 10:09:35 CST 1997  
Submit queue: Ethernet  
Submitted: 528:40:06  
Started: 528:40:06



QMS 1725 Print System

QMS 1725 (1st floor)

40/79

Warning #17 allotgem.f,452: expecting multi-dimension array - array element passed in arg #1 of SYMFAC()  
Warning #126 allotgem.f,452: different type and size used in arg #1 of SYMFAC()  
Warning #336 allotgem.f,452: different type and size used in arg #2 of SYMFAC()  
Warning #553 allotgem.f,452: different type and size used in arg #3 of SYMFAC()  
Warning #686 allotgem.f,452: different type and size used in arg #4 of SYMFAC()  
Warning #686 allotgem.f,452: different type and size used in arg #5 of SYMFAC()  
Warning #717 allotgem.f,453: expecting multi-dimension array - array element passed in arg #6 of SYMFAC()  
Warning #686 allotgem.f,453: different type and size used in arg #6 of SYMFAC()  
Warning #686 allotgem.f,453: different type and size used in arg #7 of SYMFAC()  
Warning #686 allotgem.f,453: different type and size used in arg #8 of SYMFAC()  
Warning #717 allotgem.f,453: expecting multi-dimension array - array element passed in arg #9 of SYMFAC()  
Warning #686 allotgem.f,453: different type and size used in arg #9 of SYMFAC()  
Warning #686 allotgem.f,453: different type and size used in arg #10 of SYMFAC()  
Warning #72 allotgem.f,554: common /REALNUM/ was not used in function ALLOTGEM()  
Warning #72 allotgem.f,554: common /REALSGEM/ was not used in function ALLOTGEM()  
Warning #72 allotgem.f,554: include file 'impl.h' was not used in routine ALLOTGEM()  
Warning #72 blkdtgem.f,146: common /REALNUM/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /AQUEOU/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /INPUT/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /AFFIN/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /TIMESTP/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /TO/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /TOLER/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /DAMK/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /BND/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /INIBND/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /CHAR/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /MAX/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /aqbnd/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /GASBND/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /GRAPH/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /JACMAT/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /DIFF/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /CORR/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /ELEC/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /STEP/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /QSSA/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /JINDEX/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /MASTER/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /INDICES/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /NAMINDX/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /FLUXGD/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /VARGRID/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /IONEX/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /PLT/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /PLTNDX/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /EXPAND/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /EHDAT/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /THERM/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /THERMINT/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /BREAK/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /VARPOR/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /UNITS/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /RHO/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /DEBYTAB/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /JACEXCH/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /PECNR/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /GRDSIZE/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /GHOST/ was not used in function GEMBLK()  
Warning #72 blkdtgem.f,146: common /SRCECOM/ was not used in function GEMBLK()

Warning #7 blkdtgem.f,146: include file 'i. h' was not used in routine GEMBLK()  
Warning #72 bndcond.f,353: common /REALSGEM/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /AQUEOU/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /AFFIN/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /TIMESTP/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /TO/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /TOLER/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /DAMK/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /BND/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /CHAR/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /MAX/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /OUT/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /AQBND/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /GASBND/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /GRAPH/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /JACMAT/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /DIFF/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /CORR/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /ELEC/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /STEP/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /QSSA/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /JINDEX/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /MASTER/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /INDICES/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /NAMINDX/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /FLUXGD/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /VARGRID/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /IONEX/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /PLT/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /PLTNDX/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /EXPAND/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /STOVAR/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /EHDAT/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /THERM/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /THERMINT/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /BREAK/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /VARPOR/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /UNITS/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /RHO/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /DEBYTAB/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /JACEXCH/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /PECNR/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /GRDSIZE/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /SRCECOM/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /FLOW/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /KINETIC/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /DEBYE/ was not used in function BNDCOND()  
Warning #72 bndcond.f,353: common /GAS/ was not used in function BNDCOND()  
Warning #72 cehyliq.f,172: expecting 3-dimension array - 2-dimension array passed in arg #3 of BNDCOND()  
Warning #72 cehyliq.f,400: common /ALLOCG/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /AQUEOU/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /AFFIN/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /TIMESTP/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /TO/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /TOLER/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /DAMK/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /BND/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /CHAR/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /MAX/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /OUT/ was not used in function CEHYLIQ()



Warning #72 cehyliq.f,400: common /GASBND/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /GRAPH/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /JACMAT/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /DIFF/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /CORR/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /ELEC/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /STEP/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /QSSA/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /JINDEX/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /MASTER/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /INDICES/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /NAMINDX/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /FLUXGD/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /VARGRID/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /IONEX/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /PLT/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /PLTNDX/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /EXPAND/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /STOVAR/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /EHDAT/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /THERM/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /THERMINT/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /BREAK/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /VARPOR/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /UNITS/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /DEBYTAB/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /JACEXCH/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /PECNR/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /KINETIC/ was not used in function CEHYLIQ()  
Warning #72 cehyliq.f,400: common /DEBYE/ was not used in function CEHYLIQ()

**postscript**

**JOB 917**

**UNTITLED -- /sparc20/lichtner/masstra  
ns/multiflo/mflo\_qa/gem**

**For:** lichtner  
**Date:** Thu Apr 3 16:45:20 CST 1997  
**Creator:** Edit  
**Creation Date:** Thu Apr 3 16:45:19 1997  
  
**Submit queue:** Ethernet  
**Submitted:** 535:07:52  
**Started:** 535:07:53



**QMS 1725 Print System**

**QMS 1725 (1st floor)**

44/79

c\*file maingem.f

c Program Name: MULTIFLO/GEM  
c File/Main Program Name: maingem.f  
c Release Date: February, 1997  
c Release Version: 1.0  
c Client Name: USNRC  
c Client Contact: Bret Leslie (301-415-6652)  
c Contract Number: NRC 02-93-005  
c CNWRA Contact: Peter C. Lichtner (210-522-6084)  
c Center for Nuclear Waste Regulatory Analyses  
c San Antonio, Texas 78238-5166  
c lichtner@swri.edu  
cc

c VERSION/REVISION HISTORY

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

c-----  
c Date Author(s) Comments/Modifications  
c-----  
c February 97 Peter C. Lichtner Initial Implementation  
c Mohan S. Seth  
cc

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.

**postscript**

**JOB 922**

**UNTITLED -- /sparc20/lichtner/masstra  
ns/multiflo/mflo\_qa/gem**

**For:** lichtner  
**Date:** Thu Apr 3 16:52:14 CST 1997  
**Creator:** Edit  
**Creation Date:** Thu Apr 3 16:52:13 1997

**Submit queue:** Ethernet  
**Submitted:** 535:14:33  
**Started:** 535:14:33



**QMS 1725 Print System**

**QMS 1725 (1st floor)**

program gem

\*\*\*\*\*

c  
c  
c gem is a multi-component-chemical-transport-model for  
c fluids reacting with minerals.

c  
c author ... peter c. lichtner  
c cnwra  
c southwest research institute  
c 6220 culebra road  
c san antonio, texas 78238-5166  
c

c description ... gem simulates solute transport for steady one-  
c dimensional mass transport by advection,  
c dispersion and diffusion in a saturated  
c porous medium.  
c chemical reactions incorporated in the code  
c include aqueous complexation, redox reactions,  
c precipitation/dissolution of minerals and ion  
c exchange. provision is included for both  
c reversible and irreversible reactions of minerals.  
c

c main program:  
c gemmain  
c

c subroutines:

c allotgem.f	difoft.f	gridld.f	mastrnos.f	solver.f
c blkdtgem.f	eqjac.f	gunits.f	maxchg.f	speciate.f
c bndcond.f	eqlib.f	hybrid.f	mltpsiex.f	startup.f
c cehyliq.f	eqres.f	initgem.f	modbnd.f	stdyst.f
c cehytwph.f	explicit.f	initrate.f	mprove.f	stepgem.f
c cetvdliq.f	fit.f	interp.f	opspltex.f	testgem.f
c cetvdtwp.f	fkinet.f	ionexc.f	opspltgl.f	textab.f
c cexact.f	flogk.f	kinrxn.f	opspltim.f	transp.f
c cgasos.f	fun.f	outputl.f	unitconv.f	
c cihytwph.f	gameq.f	kinrxnex.f	output2.f	updtgem.f
c cliqos.f	gamextd.f	lubksb.f	path.f	watsolv.f
c cpefrxn.f	ghostpsi.f	ludcmp.f	pecletr.f	zonek.f
c coshyliq.f	graphld.f	maingem.f	psat.f	
c dataall.f	graph2d.f	massbal.f	readat.f	
c database.f	graph3d.f	mastrnex.f	solprd.f	
c density.f	grid.f	mastrnim.f	solprodt.f	

c include files

c addgem.h	fields.h	iounits.h	ofiles.h	surfkin.h
c comgem.h	frfmt.h	kinetic.h	paramtrs.h	tempfld.h

47/79

**postscript**

**JOB 923**

**UNTITLED -- /u01/lichtner\_u01/for\_study\_analysis/gem2**

**For:** lichtner  
**Date:** Thu Apr 3 17:04:50 CST 1997  
**Creator:** Edit  
**Creation Date:** Thu Apr 3 17:04:50 1997  
  
**Submit queue:** Ethernet  
**Submitted:** 535:26:47  
**Started:** 535:26:48

48/hg

-----  
FOR\_STUDY v2.0.1 GLOBAL REPORTS - Created on 04/02/1997 at 18:35:03  
-----

Error &/or warning message(s) sent to 'msgs.rpt'

There were 0 syntax errors reported  
5 semantic errors reported  
and 3403 warnings reported in this run.

Warning #717 allotgem.f,452: expecting multi-dimension array - array  
element passed in arg #1 of SYMFAC()  
Warning #686 allotgem.f,452: different type and size used in arg #1 of  
SYMFAC()  
Warning #686 allotgem.f,452: different type and size used in arg #2 of  
SYMFAC()  
Warning #686 allotgem.f,452: different type and size used in arg #3 of  
SYMFAC()  
Warning #686 allotgem.f,452: different type and size used in arg #4 of  
SYMFAC()  
Warning #686 allotgem.f,452: different type and size used in arg #5 of  
SYMFAC()  
Warning #717 allotgem.f,453: expecting multi-dimension array - array  
element passed in arg #6 of SYMFAC()  
Warning #686 allotgem.f,453: different type and size used in arg #6 of  
SYMFAC()  
Warning #686 allotgem.f,453: different type and size used in arg #7 of  
SYMFAC()  
Warning #686 allotgem.f,453: different type and size used in arg #8 of  
SYMFAC()  
Warning #717 allotgem.f,453: expecting multi-dimension array - array  
element passed in arg #9 of SYMFAC()  
Warning #686 allotgem.f,453: different type and size used in arg #9 of  
SYMFAC()

49/79

This file was created on: Thu Apr 3 17:56:02 1997

---

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

Prepared for the U.S. NRC

Version 1.0

Enhanced Memory Version: February, 1997

MULTICOMPONENT CHEMICAL TRANSPORT MODEL

Copyright (c) 1997 Southwest Research Institute  
All Rights Reserved

---

Test Data for Multiflo Simulator (Yucca Mt., 1D, 83.4 AML)  
April 3, 1997

\*GRID--->

Co-ordinate Geometry : XYZ

```
Number of Elements in I-direction..... NX =      1
Number of Elements in J-direction..... NY =      1
Number of Elements in K-direction..... NZ =    121
Total Number of Elements..... NB =    121
Index for Mode of Operation .....MODE =      2
Index for Amount of Output ..... IPRINT =      0
Index for Debugging ..... IDEBUG =      0
```

\*OPTS

Parameters Specifying Options Invoked

```
Index for Reading Database....IDATA = 0
Index for Run Type .....ISTART = 0
Frequency of Screen Printout...IMOD = 1
Exact solution.....IEXACT = 0
Invoke scaling.....ISCALE = 0
Maximum Newtonian Iterations..ITMAX = 16
Maximum Time-Step Cuts.....IHALMAX = 16
Damping Factor .....NDAMP = 5
Index for Formulation-Method.METHOD = 1
Index for OS Algorithm.....IOPS = 0
Index for Finite-Differencing..IFOR = 2
```



Index for Mineral Surf. area..ISURF = 1  
Index for Activity Coefs.....IACT = 1  
Index for LOG/LINEAR .....LOGLIN = 0  
Index for Diffusion Constant...ICON = 1  
Courant Nr.....COURNR = 1.000

This file was created on: Thu Apr 3 17:47:16 1997

```

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

```

Prepared for the U.S. NRC

VERSION 1.0

February 1997

MULTIPHASE-MULTICOMPONENT CHEMICAL TRANSPORT MODEL

Copyright (c) 1997 Southwest Research Institute  
All Rights Reserved

Test Data for Multiflo Simulator (Yucca Mt., 1D, 83.4 AML)  
April 3, 1997

```

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

Number of Elements in I-direction..... NX =      1
Number of Elements in J-direction..... NY =      1
Number of Elements in K-direction..... NZ =     121
Total Number of Elements..... NB =     121
Index for Mode of Operation .....MODE =      2
Index for Amount of Output ..... IPRINT =      0
Index for Debugging ..... IDEBUG =      0

```

\*OPTS Parameters Specifying Options Invoked

```

Index for Reading Database....IDATA = 0
Index for Run Type .....ISTART = 0
Frequency of Screen Printout...IMOD = 1
Exact solution.....IEXACT = 0
Invoke scaling.....ISCALE = 0
Maximum Newtonian Iterations..ITMAX = 16
Maximum Time-Step Cuts.....IHALMAX = 16
Damping Factor .....NDAMP = 5
Index for Formulation-Method.METHOD = 1
Index for OS Algorithm.....IOPS = 0
Index for Finite-Differencing..IFOR = 2
Index for Mineral Surf. area..ISURF = 1
Index for Activity Coefs.....IACT = 1
Index for LOG/LINEAR .....LOGLIN = 0

```

Index for Diffusion Constant...ICON = 1  
Courant Nr.....COURNR = 1.000

pcl4

JOB 858

msgs.rpt

*Executive*

*Analysis Results for  
Running of FOR-STUDY  
for Executive*

*Gen  
4/3/97*

For: root  
Date: Thu Apr 3 10:07:58 CST 1997  
Submit queue: Ethernet  
Submitted: 528:38:32  
Started: 528:38:32



QMS 1725 Print System

QMS 1725 (1st floor)

```
Warning #700 gem.f,192: No interface for routine READAT()
Warning #700 gem.f,194: No interface for routine ALLOTGEM()
Warning #700 gem.f,200: No interface for routine GRID1D()
Warning #700 gem.f,202: No interface for routine GRID()
Warning #700 gem.f,208: No interface for routine INITGEM()
Warning #700 gem.f,351: No interface for routine OUTPUT1()
Warning #700 gem.f,358: No interface for routine OUTPUT2()
Warning #700 gem.f,421: No interface for routine MASTRNIM()
Warning #700 gem.f,429: No interface for routine MASTRNOS()
Warning #700 gem.f,440: No interface for routine MASTRNEX()
Warning #700 gem.f,445: No interface for routine UPDTGEM()
Warning #700 gem.f,458: No interface for routine PECLETNR()
Warning #712 gem.f,507: expecting scalar argument - not entire array in arg #1 of DTIME()
Error #177 gem.f,566: Local name TYME was referenced but never set
Warning #72 gem.f,566: common /AQUEOU/ was not used in function GEM()
Warning #72 gem.f,566: common /AFFIN/ was not used in function GEM()
Warning #72 gem.f,566: common /TO/ was not used in function GEM()
Warning #72 gem.f,566: common /TOLER/ was not used in function GEM()
Warning #72 gem.f,566: common /DAMK/ was not used in function GEM()
Warning #72 gem.f,566: common /BND/ was not used in function GEM()
Warning #72 gem.f,566: common /CHAR/ was not used in function GEM()
Warning #72 gem.f,566: common /MAX/ was not used in function GEM()
Warning #72 gem.f,566: common /OUT/ was not used in function GEM()
Warning #72 gem.f,566: common /AQBND/ was not used in function GEM()
Warning #72 gem.f,566: common /GASBND/ was not used in function GEM()
Warning #72 gem.f,566: common /GRAPH/ was not used in function GEM()
Warning #72 gem.f,566: common /DIFF/ was not used in function GEM()
Warning #72 gem.f,566: common /CORR/ was not used in function GEM()
Warning #72 gem.f,566: common /ELEC/ was not used in function GEM()
Warning #72 gem.f,566: common /QSSA/ was not used in function GEM()
Warning #72 gem.f,566: common /JINDEX/ was not used in function GEM()
Warning #72 gem.f,566: common /MASTER/ was not used in function GEM()
Warning #72 gem.f,566: common /INDICES/ was not used in function GEM()
Warning #72 gem.f,566: common /NAMINDX/ was not used in function GEM()
Warning #72 gem.f,566: common /FLUXGD/ was not used in function GEM()
Warning #72 gem.f,566: common /VARGRID/ was not used in function GEM()
Warning #72 gem.f,566: common /IONEX/ was not used in function GEM()
Warning #72 gem.f,566: common /PLTNDX/ was not used in function GEM()
Warning #72 gem.f,566: common /STOVAR/ was not used in function GEM()
Warning #72 gem.f,566: common /EHDAT/ was not used in function GEM()
Warning #72 gem.f,566: common /THERM/ was not used in function GEM()
Warning #72 gem.f,566: common /THERMINT/ was not used in function GEM()
Warning #72 gem.f,566: common /BREAK/ was not used in function GEM()
Warning #72 gem.f,566: common /VARPOR/ was not used in function GEM()
Warning #72 gem.f,566: common /UNITS/ was not used in function GEM()
Warning #72 gem.f,566: common /DEBYTAB/ was not used in function GEM()
Warning #72 gem.f,566: common /JACEXCH/ was not used in function GEM()
Warning #72 gem.f,566: common /PECNR/ was not used in function GEM()
Warning #72 gem.f,566: common /GRDSIZE/ was not used in function GEM()
Warning #72 gem.f,566: common /GHOST/ was not used in function GEM()
Warning #72 gem.f,566: common /SRCECOM/ was not used in function GEM()
Warning #72 gem.f,566: common /CXKIN/ was not used in function GEM()
Warning #72 gem.f,566: common /MINRL/ was not used in function GEM()
Warning #72 gem.f,566: common /GAS/ was not used in function GEM()
Warning #72 gem.f,566: common /KINETIC/ was not used in function GEM()
Warning #72 gem.f,566: common /SURFKIN/ was not used in function GEM()
Warning #72 gem.f,566: common /DEBYE/ was not used in function GEM()
Warning #72 gem.f,566: common /SCRATCH/ was not used in function GEM()
Warning #72 gem.f,566: common /OPENF/ was not used in function GEM()
Warning #72 gem.f,566: include file 'gem/scratch.h' was not used in routine GEM()
```

```
Warning #72 gem.f,566: include file 'gem/ofc_s.h' was not used in routine GEM()
Warning #72 gem.f,653: common /REALNUM/ was not used in function SETVEL()
Warning #72 gem.f,653: common /IOUNITS/ was not used in function SETVEL()
Warning #72 gem.f,653: common /AQUEOU/ was not used in function SETVEL()
Warning #72 gem.f,653: common /INPUT/ was not used in function SETVEL()
Warning #72 gem.f,653: common /AFFIN/ was not used in function SETVEL()
Warning #72 gem.f,653: common /TO/ was not used in function SETVEL()
Warning #72 gem.f,653: common /TOLER/ was not used in function SETVEL()
Warning #72 gem.f,653: common /DAMK/ was not used in function SETVEL()
Warning #72 gem.f,653: common /BND/ was not used in function SETVEL()
Warning #72 gem.f,653: common /CHAR/ was not used in function SETVEL()
Warning #72 gem.f,653: common /MAX/ was not used in function SETVEL()
Warning #72 gem.f,653: common /OUT/ was not used in function SETVEL()
Warning #72 gem.f,653: common /AQBND/ was not used in function SETVEL()
Warning #72 gem.f,653: common /GASBND/ was not used in function SETVEL()
Warning #72 gem.f,653: common /GRAPH/ was not used in function SETVEL()
Warning #72 gem.f,653: common /JACMAT/ was not used in function SETVEL()
Warning #72 gem.f,653: common /DIFF/ was not used in function SETVEL()
Warning #72 gem.f,653: common /CORR/ was not used in function SETVEL()
Warning #72 gem.f,653: common /ELEC/ was not used in function SETVEL()
Warning #72 gem.f,653: common /STEP/ was not used in function SETVEL()
Warning #72 gem.f,653: common /QSSA/ was not used in function SETVEL()
Warning #72 gem.f,653: common /JINDEX/ was not used in function SETVEL()
Warning #72 gem.f,653: common /MASTER/ was not used in function SETVEL()
Warning #72 gem.f,653: common /INDICES/ was not used in function SETVEL()
Warning #72 gem.f,653: common /NAMINDX/ was not used in function SETVEL()
Warning #72 gem.f,653: common /FLUXGD/ was not used in function SETVEL()
Warning #72 gem.f,653: common /VARGRID/ was not used in function SETVEL()
Warning #72 gem.f,653: common /IONEX/ was not used in function SETVEL()
Warning #72 gem.f,653: common /PLT/ was not used in function SETVEL()
Warning #72 gem.f,653: common /PLTNDX/ was not used in function SETVEL()
Warning #72 gem.f,653: common /EXPAND/ was not used in function SETVEL()
Warning #72 gem.f,653: common /STOVAR/ was not used in function SETVEL()
Warning #72 gem.f,653: common /EHDAT/ was not used in function SETVEL()
Warning #72 gem.f,653: common /THERM/ was not used in function SETVEL()
Warning #72 gem.f,653: common /THERMINT/ was not used in function SETVEL()
Warning #72 gem.f,653: common /BREAK/ was not used in function SETVEL()
Warning #72 gem.f,653: common /VARPOR/ was not used in function SETVEL()
Warning #72 gem.f,653: common /UNITS/ was not used in function SETVEL()
Warning #72 gem.f,653: common /DEBYTAB/ was not used in function SETVEL()
Warning #72 gem.f,653: common /JACEXCH/ was not used in function SETVEL()
Warning #72 gem.f,653: common /GRDSIZE/ was not used in function SETVEL()
Warning #72 gem.f,653: common /GHOST/ was not used in function SETVEL()
Warning #72 gem.f,653: common /SRCECOM/ was not used in function SETVEL()
Warning #72 gem.f,653: common /FLOW/ was not used in function SETVEL()
Warning #72 gem.f,653: include file 'metra/impl.h' was not used in routine SETVEL()
Warning #72 gem.f,653: include file 'gem/iounits.h' was not used in routine SETVEL()
Warning #72 gem.f,653: include file 'gem/fields.h' was not used in routine SETVEL()
Warning #72 mainmlti.f,323: expecting scalar argument - not entire array in arg #1 of DTIME()
Warning #72 mainmlti.f,341: No interface for routine GUNITS()
Warning #72 mainmlti.f,346: function FDATE() return type differs with interface
Warning #72 mainmlti.f,444: No interface for routine ALLOT()
Warning #72 mainmlti.f,524: expecting scalar argument - not entire array in arg #1 of DTIME()
Error #72 mainmlti.f,571: Local name TYME was referenced but never set
Warning #72 mainmlti.f,571: common /AQUEOU/ was not used in function MULTIFLO()
Warning #72 mainmlti.f,571: common /AFFIN/ was not used in function MULTIFLO()
Warning #72 mainmlti.f,571: common /TO/ was not used in function MULTIFLO()
Warning #72 mainmlti.f,571: common /TOLER/ was not used in function MULTIFLO()
Warning #72 mainmlti.f,571: common /DAMK/ was not used in function MULTIFLO()
Warning #72 mainmlti.f,571: common /BND/ was not used in function MULTIFLO()
```

Warning #72 mainm1ti.f,571: common /INIBND/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /CHAR/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /MAX/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /OUT/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /AQBND/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /GASBND/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /GRAPH/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /JACMAT/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /DIFF/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /CORR/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /ELEC/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /STEP/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /QSSA/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /JINDEX/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /MASTER/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /INDICES/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /NAMINDX/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /FLUXGD/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /VARGRID/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /IONEX/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /PLTNDX/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /EXPAND/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /STOVAR/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /EHDAT/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /THERM/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /THERMINT/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /BREAK/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /VARPOR/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /UNITS/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /RHO/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /DEBYTAB/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /JACEXCH/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /PECNR/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /GRDSIZE/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /GHOST/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /SRCECOM/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /FLOW/ was not used in function MULTIFLO()  
Warning #72 mainm1ti.f,571: common /OPENF/ was not used in function MULTIFLO()  
Warning #9 mainm1ti.f,571: include file 'gem/fields.h' was not used in routine MULTIFLO()  
Warning #9 mainm1ti.f,571: include file 'gem/ofiles.h' was not used in routine MULTIFLO()  
Warning #72 mainm1ti.f,714: common /REALNUM/ was not used in function FRFMT()  
Warning #9 mainm1ti.f,714: include file 'metra/impl.h' was not used in routine FRFMT()  
Warning #72 mainm1ti.f,829: common /REALNUM/ was not used in function CPUTIM()  
Warning #72 mainm1ti.f,829: common /CHRS/ was not used in function CPUTIM()  
Warning #9 mainm1ti.f,829: include file 'metra/impl.h' was not used in routine CPUTIM()  
Warning #700 mainm1ti.f,852: No interface for routine ETIME()  
Warning #700 metra.f,375: No interface for routine OPENFLS()  
Warning #700 metra.f,427: No interface for routine RSTART()  
Warning #700 metra.f,440: No interface for routine INPMETRA()  
Warning #700 metra.f,452: No interface for routine INIT()  
Warning #700 metra.f,455: No interface for routine PVTH20()  
Warning #700 metra.f,486: No interface for routine RECDAT()  
Warning #700 metra.f,504: No interface for routine AUTODT()  
Warning #700 metra.f,513: No interface for routine SETBC()  
Warning #700 metra.f,519: No interface for routine ITER()  
Warning #700 metra.f,521: No interface for routine PVT()  
Warning #700 metra.f,522: No interface for routine ACCM()  
Warning #700 metra.f,522: No interface for routine COEFS()  
Warning #700 metra.f,522: No interface for routine UPDTPSK()  
Warning #700 metra.f,527: No interface for routine PVTVP()

57/79

Warning #700 metra.f,528: No interface for routine ACCMVP()  
Warning #700 metra.f,528: No interface for routine COEFSVP()  
Warning #700 metra.f,528: No interface for routine UPDTVPK()  
Warning #700 metra.f,532: No interface for routine COND()  
Warning #700 metra.f,536: No interface for routine SLVLIQ()  
Warning #700 metra.f,542: No interface for routine AUTOSTEP()  
Warning #700 metra.f,555: No interface for routine UPDATE()  
Warning #700 metra.f,560: No interface for routine OUTMETRA()  
Warning #72 metra.f,612: common /COM2/ was not used in function METRA()  
Warning #72 metra.f,612: common /COMBC/ was not used in function METRA()  
Warning #72 metra.f,612: common /PVTTAB/ was not used in function METRA()  
Warning #72 metra.f,612: common /RELP/ was not used in function METRA()  
Warning #9 metra.f,612: include file 'metra/pvttbl.h' was not used in routine METRA()  
Warning #9 metra.f,612: include file 'metra/pckr.h' was not used in routine METRA()



## **SCIENTIFIC NOTEBOOK INFORMATION**

58/75

Printed: April 3, 1997

P. C. Lichtner

## SCIENTIFIC NOTEBOOK

INITIALS: PCZAccount Number: **20-5708-562**

Description: Near-field Environment Code Development – MULTIFLO

Collaborators: Dr. M. Seth (Consultant)

**Objective:** Development of the computer code MULTIFLO, and submodules GEM and METRA.

**DATE****4.3.97 QA Installation Test of MULTIFLO.**

To meet QA TOP-018 requirements an Installation Test of MULTIFLO was performed. The code was compiled and run on the machine `hornet.cnwra.swri.edu`, an ultra-sparc machine. The results were compared with those obtained from running the code on `skippy.cnwra.swri.edu`, a sparc 20 machine. Slight differences are expected due to the different machine types. The input files used in the test are listed below for metra and gem:

METRA Data for Multiflo simulator (initial data:1D, 83.4 AML, Yucca Mt.)  
Apr. 3, 1997

```
RSTART 0
:
:      XYZ              = 1 table look-up, pref = ref. press.
:      RADIAL           = 0 correlations,   tref = ref temp.
:      OTHER
:grid geometry nx ny nz ivplwr ipvcal iout gravity pref tref href
Grid XYZ      1  1 121  1    0    3    0    0    0    0
:
Pckr                                :relative perm and pc keyword
:  1 type-curv swirm rpmm(lamda) alpham swext sgc iecm
:      swirf rpmf(lamda) alphaf phim phif permf permf
:Topopah Spring (150-475 m)
:  1 Van-Gen  0.08  0.4400  5.8e-7  0.  0.  1
:      0.04  0.7636  1.305e-5 0.11  1.8e-3 1.9e-18 3.9e-12
:  1 Van-Gen  0.001 0.4400  5.8e-7  0.  0.  1
:      0.001 0.7636  1.305e-5 0.11  1.8e-3 1.9e-18 3.9e-12
:  1 Van-Gen  0.001 0.4400  5.8e-7  0.  0.  1
:      0.001 0.7636  1.305e-5 0.11  1.8e-3 1.9e-18 1.0e-11
:blank line
:
Thermal-prop
: no rho      cpr  ckdry cksat  crp crt  tau cdiff  cexp enbd
:  1 2.580e+3 840.  2.10  2.10    0    0    .5 2.13e-5 1.8 0.
0
:  igrd  rw      re
DXYZ  0      0.    1.
: (dx(i),i=1,nx)
```

59/79

Printed: April 3, 1997

P. C. Lichtner

## SCIENTIFIC NOTEBOOK

INITIALS: PCZ

```

1.
:
: (dy(j),j=1,ny)
1.
:
: (dz(k),k=1,nz)
10. 10. 10. 10. 10. 10. 10. 10. 10. 10.
10. 10. 10. 10. 10. 10. 10. 10. 10. 10.
10. 10. 10. 10. 5. 5. 5. 5. 5. 5.
5. 5. 5. 5. 5. 5. 5. 5. 5. 5.
2. 2. 2. 2. 2. 2. 2. 2. 2. 2.
2. 2. 2. 2. 2. 2. 2. 2. 2. 2.
2. 2. 2. 1.5 1. 1. 1. 1. 1. 1.
1. 1. 1. 1. 1. 1. 1. 1. 1. 1.5
2. 2. 2. 2. 2. 2. 2. 2. 2. 2.
2. 2. 2. 2. 2. 2. 2. 2. 5. 5.
5. 5. 5. 5. 5. 5. 5. 5. 10. 10.
10. 10. 10. 10. 10. 10. 10. 10. 10. 10.
10.
PhiK
: i1 i2 j1 j2 k1 k2 iist ithrm vb porm permx permy permz
  1 1 1 1 1 121 1 1 0.
0
Init init
: i1 i2 j1 j2 k1 k2 pm tm sgm x2m
: 1 1 1 1 1 121 1.e5 25.0 0.5 0.
: 0
:
:EQUIL 587.50 1.e5 30. 0.0255319 0.0 -1
:EQUIL 5.0 1.e5 25. 0. 0.2 1
:EQUIL 595.0 1.065627E+05 25. 0.0 0.0 -1
:
Recurrent-data
Bcon 2
:itype iface i1 i2 j1 j2
1 TOP 1 1 1 1
:time qbc pbc tbc sgbc xabc
0. 0. 8.55e4 15.0 0.2 0.
0
1 BOTTOM 1 1 1 1
0. 0. 9.05e4 30.0 0.0 0.
0
:
Rstart 1 0
Output A=1 C=1 B=1 S=-1
: isolve newtnmn newtnmx north nitmx level
Solve 2 1 7 4 100 1
:
:AUTO-step DPMXE DSMXE DTMPMXE DP2MXe TACCEL IAUTODT FAC1
AUTO-step 1.0E+3 0.03 5.0 1.e3 1.e-3 0 0
:
:TOLR TOLP TOLS TOLT TOLP2 TOLM TOLA TOLE rtwotol rmxtol smxtol
Tolr 10. 1.e-4 1.e-3 1.e+1 1.e-5 1.e-3 1.e-3 1.e-20 1.e-20 1.e-20

```

60/79

Printed: April 3, 1997

P. C. Lichtner

## SCIENTIFIC NOTEBOOK

INITIALS: SCZ

```

:
:Limit dpmx      dsmx dtmpmx dp2mx dtmn dtmx icutmx
LIMIT 1.e4      .08    10.    1.e5  1.e-6 1.e3
Plots 1
:Steady[y] 1.e-8 1.e-6 1.e-1
:Ends
:      ns      fach      facm (fach and facm are multipliers to
:                        read-in values of qht and qmt)
:Source 1 1.32494 1. !110.5 AML
:Source 1 1.19904 1. !100 AML
:Source 1 1.13909 1. ! 95 AML
:Source 1 1.07914 1. ! 90 AML
:Source 1 1.04916 1. ! 87.5 AML
:Source 1 1.01918 1. ! 85 AML
Source 1 1. 1. ! 83.4 AML
:Source 1 3.14159 1. !radial 83.4 AML
: is js ks istyp
  1 1 1 1 72 72 31
: 1 1 1 1 72 72 33
: timeq(sec) T/qht (C/(J/s)) qmt (kg/s)
0.00000E+00 1.87730E+01
6.30720E+07 1.81217E+01
1.26144E+08 1.75357E+01
1.89216E+08 1.68897E+01
2.52288E+08 1.63046E+01
3.15360E+08 1.57715E+01
4.73040E+08 1.45818E+01
6.30720E+08 1.34618E+01
7.88400E+08 1.25071E+01
9.46080E+08 1.16163E+01
1.26144E+09 1.02515E+01
1.57680E+09 8.99586E+00
2.36520E+09 6.82702E+00
3.15360E+09 5.65219E+00
4.73040E+09 4.24896E+00
6.30720E+09 3.53303E+00
9.46080E+09 2.82589E+00
1.26144E+10 2.40733E+00
1.57680E+10 2.08456E+00
1.89216E+10 1.81067E+00
2.52288E+10 1.44680E+00
3.15360E+10 1.20944E+00
3.94200E+10 9.81818E-01
4.73040E+10 8.27487E-01
6.30720E+10 6.33691E-01
7.88400E+10 5.48998E-01
9.46080E+10 4.89297E-01
1.26144E+11 4.38708E-01
1.57680E+11 4.02873E-01
1.89216E+11 3.70297E-01
2.20752E+11 3.44801E-01
2.52288E+11 3.24128E-01
2.83824E+11 3.06917E-01

```

61/79

Printed: April 3, 1997

P. C. Lichtner

## SCIENTIFIC NOTEBOOK

INITIALS: PCZ

```

3.15360E+11 2.92001E-01
3.46896E+11 2.69319E-01
3.78432E+11 2.50151E-01
4.09968E+11 2.33722E-01
4.41504E+11 2.19473E-01
4.73040E+11 2.06987E-01
5.51880E+11 1.81593E-01
6.30720E+11 1.62125E-01
7.88400E+11 1.34131E-01
9.46080E+11 1.14855E-01
1.26144E+12 8.27996E-02
1.57680E+12 6.29212E-02
1.89216E+12 4.90735E-02
2.20752E+12 3.97719E-02
2.52288E+12 3.31523E-02
2.83824E+12 2.82343E-02
3.15360E+12 2.44608E-02
4.73040E+12 1.84539E-02
0
Output  A=1  C=1  S=-1
:
:RStArt 0 1
:
:  isolv  newtnmn  newtnmx
Solve 3      2      7
:
:AUtO-step  DPMXE      DSMXE DTMPMXE DP2MXe TACCEL IAUTO
AUtO-step  5.E+4  0.025  3.0  1.e4      1.e-2  0
:
:TOLR TOLP  TOLS  TOLT  TOLP2  TOLM  TOLA  TOLE
Tolr  1.e+1 1.e-4 1.e-2 5.e+1 1.e-5 1.e-6 1.e-3 1.e-20 1.e-20 1.e-12
:
:Limit dpmx  dsmx  dtmpmx  dp2mx  dtmn  dtmx  icutmx
LIMIT 1.e4  .05  5.  1.e5  1.e-6  1.e4  5
Plots 1 1 1
72
Time[y] 10.
Time[y] 50.
Time[y] 100.
Time[y] 500.
Time[y] 1000.
Time[y] 5000.
Time[y] 10000.
Time[y] 1.e5
:Time[y] 1.5e5
Ends

```

GEM Test Data for Multiflo Simulator (Yucca Mt., 1D, 83.4 AML)

Apr. 3, 1997

```

:
:      geometry nx  ny  nz      mode  iprint idebug
GRID   XYZ      1   1 121      2      0      0
:

```

62/75

Printed: April 3, 1997

P. C. Lichtner

## SCIENTIFIC NOTEBOOK

INITIALS: SC

```

OPTS
:  idata istart imod iexact iscale
    0      0      1      0      0
:
:  itmax ihalmax ivmax ndamp
    16     16     0      5
:
:  method iops  ifor   isurf iact  loglin  icon   counr
    1      0      2      1      1      0      1      1.
:
:      isync ipor iperm perm-fac.
COUPLE 0      -1      0      3.
:
PLTFiles
:iplot  a  s  t  m  s  i  s  f  v  z  b  i  n  e  e  x  t  i  g  i  t  e  x
    1  1  1  1  1  0  0  1  0  2  0  0  0  0  1  0
:
:      tol  ttol  tolneg tolpos tolexp  dthalf qkmax tolstdste tolc
TOLR 1.d-10 2.e-3 1.e0 1.e-2 5.d0  .5  590.  1.e-12 1.e-10
:
:      mcyc cc  c  flx r  sp  qk  pk  rk  a1  a2  a3
DEBUG 0      1  1  0  1  1  1  1  1  1
:
:      isat isotherm iread por0 phir sat  w  lambda toldelt tolpor
ISYSem 0      1      0  .11  1.  0.5  .5  1.  1.e-3 1.e-3
:
:      vx0 vy0 vz0 vgx0 vgy0 vgz0[m/yr] alphax  alphay  alphaz[m]
FLOW 0.  0.  1.  0.  0.  0.  0.  0.  0.  0.
:
:      d0[cm^2/s] delhaq[kJ/mol] dgas[cm^2/s] dgexp tortaq tortg idif
DIFF 1.d-5  12.6  2.13d-1  1.8  1.d0  1.d0  0
:
:flag 1: T(x) = d x^3 + a x^2 + b x + c (meters)
:      2: T(x) = a + (b-a) exp[-((x-x0)/c)^2] + (d - a) * x / xlen
:      3: T(x,t)=a+1/2(b-a)(erf[(x+c-x0)/2sqr(dt)]-erf[(x-c-x0)/2sqr(dt)])
:      p (bars) temp flag a  b  c  d  x0  xlen
PTINit 1.e5  25.  0  25  300  250  125  1000.  2.d3
:
:master species for controlling time stepping
MASTER h+
:
:grid m 0. 1 200 200.
:
DXYZ
    1.
    1.
    121*1.
:
:  isolv level north nitmax idetail rmaxtol rtwotol smaxtol
SOLV 3  1  1  100  0  1.e-20 1.e-20 1.e-12
:
:initial and boundary conditions: 1-conc., 2-flux, 3-zero gradient
:inlet outlet nzoneaq

```

63/79

Printed: April 3, 1997

P. C. Lichtner

# SCIENTIFIC NOTEBOOK

INITIALS: SCZ

```

COMP      1      3      3
:
:species itype guess ctot mineral diffusion
ca+2      1      4.e-4  2.5e-3  blank
mg+2      1      1.e-4  7.8e-4  blank
na+       1      2.e-3  3.0e-3  blank
k+        1      2.e-4  3.6e-4  blank
h+        3      1.e-8   8.2      calcite
hco3-     4      2.7e-3 -2.00    co2(g)
sio2(aq)  1      1.e-3  1.5e-3  blank
cl-       -1     2.e-3  2.8e-3  blank
so4-2     1      3.e-4  1.7e-3  blank
:o2(aq)   4      1.e-3   0.2      o2(g)
      :blank
:
BCON
      3      1
:species itype guess ctot mineral
ca+2      1      4.e-4  2.5e-3  blank
mg+2      1      1.e-4  7.8e-4  blank
na+       1      2.e-3  3.0e-3  blank
k+        1      2.e-4  3.6e-4  blank
h+        3      1.e-8   8.2      calcite
hco3-     4      2.7e-3 -2.00    co2(g)
sio2(aq)  1      1.e-3  1.5e-3  blank
cl-       -1     2.e-3  2.8e-3  blank
so4-2     1      3.e-4  1.7e-3  blank
:o2(aq)   4      1.e-3   0.2      o2(g)
:
      4      1
:species itype guess ctot mineral
ca+2      1      4.e-4  2.5e-4  blank
mg+2      1      1.e-4  7.2e-5  blank
na+       1      2.e-3  1.96e-3  blank
k+        1      2.e-4  1.36e-4  blank
h+        8      1.e-7   6.9      calcite
hco3-     -1     2.3e-3 -2.00    co2(g)
sio2(aq)  1      1.e-3  1.07e-3  blank
cl-       1      2.e-4  1.8e-4  blank
so4-2     1      3.e-4  1.9e-4  blank
:o2(aq)   7      1.e-4  1.74e-4  blank
:
      0      0
:
CMIR      0      0
      :blank
:
: 9 entries per line
STOL 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
:
AQCX
oh-
hso4-

```

64/79

Printed: April 3, 1997

P. C. Lichtner

## SCIENTIFIC NOTEBOOK

INITIALS: PCZ

```

hcl(aq)
co2(aq)
co3-2
caco3(aq)
cahco3+
caoh+
cac1+
cac12(aq)
caso4(aq)
mgoh+
mgco3(aq)
mgcl+
mghco3+
mgso4(aq)
nahco3(aq)
nacl(aq)
naoh(aq)
naso4-
kcl(aq)
khso4(aq)
kso4-
h3sio4-
h2sio4-2
      :blank
:
MNRL
quartz
calcite
tobermorite-14a
      :blank
:
GASEs
co2(g)
:o2(g)
      :blank
:
MNIR
:mineral itypkin fkin delh beta rka  betb rkb rk  tau
:i1 i2 j1 j2 k1 k2  vol  area
quartz      0  1.0  75.  1.0  0.    1.0  0. -17.39  1.e-3
1 1 1 1 1 121  0.89  1.e1
0
calcite      0  1.0  35.  1.0  0.    1.0  0. -10.00  1.e-4
1 1 1 1 1 121  0.    1.
0
      :blank
:
:surface mineral itypkin area beta  fkin  delh  rkph  rk
:    0  1.0  1.0    1.  0.    0.    0.
:
:corrosion solids i0  acorr  bcorr  curlim
:    0.  0.  0.  0.
:

```



65/79

Printed: April 3, 1997

P. C. Lichtner

## SCIENTIFIC NOTEBOOK

INITIALS: SCZ

```
:crevice gap[meters] potential [v]
ECAQ      90.d-6      -.2
          :blank
:
:electrochemical aqueous species i0   acorr   bcorr   curlim
:      0.  0.  0.  0.
:
AQIR
          :blank
:
:ion-exchange reactions
Ionx      0      1.0
:
BRKP      1
72
:
DTStep[y]      1 3.e-8
1.e-8          100.d0
:
TIME[y] 1 10. 50. 100. 500. 1000. 5000. 10000. 1.e5
:
ENDS
```

Only slight differences (4th decimal place) were found in the masout file. No differences were found in the plot files. The Installation Test was deemed successful.

**SOFTWARE  
REQUIREMENTS  
DESCRIPTION**

# SOFTWARE REQUIREMENTS DESCRIPTION

FOR THE CODE MULTIFLO

by


*Peter C. Lichtner*

CNWRA  
San Antonio, Texas

Completed April 25, 1995

**Version 1.0**

Approved by:

A handwritten signature in black ink, appearing to read 'N. Sridhar', is written over a horizontal line.

Narasi Sridhar, Manager EBS Element  
CNWRA

## Contents

1	INTRODUCTION . . . . .	1
2	SOFTWARE REQUIREMENT DESCRIPTION (SRD): MULTIFLO . . . . .	2
2.1	Software Function . . . . .	2
2.2	Theoretical Basis: Physical and Mathematical Model . . . . .	2
2.3	Computational Approach . . . . .	3
2.4	Data Flow and User Interface . . . . .	4
2.4.1	Initial and Boundary Conditions . . . . .	5
2.4.2	I/O . . . . .	5
2.5	Hardware and Software Requirements . . . . .	5
2.6	Graphics . . . . .	6
2.7	Pre- and Post-Processors . . . . .	6
3	REFERENCES . . . . .	6

## List of Tables

1	Processes-icode parameter. . . . .	5
---	------------------------------------	---

## List of Figures

1	Flow diagram for the computer code <b>MULTIFLO</b> . . . . .	7
---	--	---

---

## 1. INTRODUCTION

This Software Requirements Description (SRD) document accounts for the first stage in development of the computer code **MULTIFLO**, a numerical model describing multiphase, multicomponent, reactive transport in a partially saturated porous medium. This software will be used in the HLW repository license application review process for Yucca Mountain (YM).

Several Key Technical Uncertainties (KTUs) related to the very-near-field, and near-field relevant to the performance of the Engineered Barrier System (EBS) will be addressed by the code **MULTIFLO**. These include:

- (i) Isothermal and non-isothermal liquid and vapor phase movement of water through unsaturated rock at YM.
- (ii) Predicting the evolution of groundwater conditions near and within the engineered barrier system.
- (iii) Predicting changes in porosity and permeability of the host rock resulting from mineral alteration and their effect on fluid transport.
- (iv) Prediction of releases of non-gaseous and gaseous radionuclides from the waste package during containment and post-containment periods.

## 2. SOFTWARE REQUIREMENT DESCRIPTION (SRD): MULTIFLO

This SRD briefly outlines the software function, technical basis, computational approach, program flow and user interface, hardware and software requirements, graphics, and pre- and post-processors that are relevant to the development and use of the code **MULTIFLO**.

### 2.1. Software Function

The code **MULTIFLO** will be used to model the near-field and very-near-field environment of a HLW repository emplaced under partially saturated conditions that occur at the proposed repository at Yucca Mountain, Nevada. **MULTIFLO** describes multiphase, multicomponent, reactive transport in a partially saturated porous medium. The code **MULTIFLO** can be applied to both repository-scale and waste package scale models describing redistribution of heat, moisture, and chemical constituents in aqueous, gas and solid phases. The code will allow calculation of temperature, pressure, aqueous and gas solution compositions, saturation state, mineral abundances, porosity, permeability, and tortuosity as functions of time and space. Because of the transitory behavior of the near-field and very-near-field environments, coupling of the various processes involved is essential. Electrochemical corrosion processes are also included in the model through the code **GEM** (Lichtner, 1994b), a submodule of **MULTIFLO**. Possible mechanical effects resulting from the thermal perturbation produced by the HLW and chemical reaction are not included in **MULTIFLO**.

### 2.2. Theoretical Basis: Physical and Mathematical Model

Fundamental to a quantitative description of corrosion processes involved in the degradation of a HLW package is the specification of environmental variables defining the oxidation state, pH, chloride concentration, and other compositional variables of ingressing fluid which may impact the waste container and waste form. Interaction between groundwater and the EBS may include a diverse set of processes involving the near-field region as well as the EBS itself. Heat produced by radioactive decay of the HLW may produce a dry-out zone surrounding the repository. As a consequence, liquid water initially occupying the pore spaces in the vicinity of the repository will be transported away and could recondense some distance above and below the repository horizon. Formation of heat-pipes may aid in the heat transfer process. Water above the repository has the potential to drip or flow along fractures back to the EBS and interact with the waste package. Continued evaporation/condensation could result in the formation of a high ionic strength aqueous solution (brine), which if contacted by the waste package, could accelerate corrosion processes. Salts could form both on the waste package and in the near field as a result of evaporation. Degradation of grout could result in the formation of hyperalkaline fluids which would react strongly with the silicate host rock producing calcium silicate hydrates and affect the sorption characteristics of the near field. As the waste package cools, eventual rewetting of the EBS may occur, as the host rock returns to its initial saturation state.

The redox state of the environment contacting the EBS will be a determining factor for corrosion processes. In the absence of radiolysis effects, the redox state could be affected by competition between consumption of oxygen by oxidation reactions and supply by transport from the atmosphere. Corrosion of the waste package under oxidizing conditions will result in formation of iron-oxides and other iron-rich solids such as silicates. These reactions are accompanied by a large positive volume change which could further accelerate the corrosion process due to spalling, or halt it by formation of protective layers. Likewise dissolution and alteration of spent fuel under oxidizing conditions are likely to result in the formation of uranyl silicate minerals accompanied by a positive

volume change leading to spalling and the further release of soluble radionuclides. Formation of soluble corrosion products will affect the composition of the groundwater such as redox state, pH, and ionic strength, and thereby affect the adsorption of important radionuclides. Co-precipitation and adsorption of radionuclides will compete with other soluble oxidation products of the EBS.

Finally, mineral alteration in the near field could affect the adsorption characteristics of the EBS environs. Formation of secondary porosity, tortuosity and permeability due to mineral precipitation and dissolution at elevated temperatures could enhance reflux of liquid water to the EBS.

The purpose of computer code **MULTIFLO** is to address these issues through a fundamental description based on a system of governing partial differential equations of heterogeneous and homogeneous chemical reactions coupled to flow and transport processes in partially saturated porous media. The theoretical basis for the governing equations to be solved by **MULTIFLO** is described in detail by Lichtner (1994a, b), Lichtner and Walton (1994), and Walton and Lichtner (1995). These equations are not discussed further in this report.

The code **MULTIFLO** consists of three basic flow and transport modules:

- Solute transport and chemical reaction are described by incorporating the computer code **GEM** (Lichtner, 1994b) as a submodule in **MULTIFLO**. The code **GEM** accounts for multicomponent transport of solutes in a partially saturated porous medium taking into account electromigration of aqueous species, aqueous complexing, mineral precipitation/dissolution, electrochemical reactions, and ion-exchange and sorption reactions.
- Flow in partially saturated porous media is described by a two-phase transport module. The van Genuchten phenomenological equations are used to relate capillary pressure and liquid saturation, and provide relative permeabilities of liquid and gas phases. The equation of state for pure water extends to well over 1000°C. This will be useful for modeling moisture redistribution following dike emplacement and volcanic related processes.
- Energy conservation.

These modules are coupled through heat and mass transport, and through changes in the host rock composition resulting from chemical reactions. Mineral alteration resulting from precipitation and dissolution causes changes in porosity, permeability and tortuosity which, in turn, alters the flow field.

### 2.3. Computational Approach

The computational approach used in **MULTIFLO** consists of a finite difference approximation to the governing partial differential equations. For the most part the technical basis for the code **MULTIFLO** is well known and uses standard techniques and practices from the literature (e.g. Pruess, 1987; Nitao, 1990; Zyvoloski et al., 1992). For example, a Newton-Raphson algorithm is used to solve coupled systems of non-linear algebraic equations. Standard solvers are used to obtain solutions to the resulting linearized equations. The modules used to describe two-phase fluid flow and energy conservation are similar to the code **CTOUGH**.

After careful consideration it was decided not to modify **CTOUGH** and incorporate it into **MULTIFLO**, but rather to construct an entirely new algorithm. There were several reasons for this decision:

- (i) Modification of **CTOUGH** would require essentially the same effort as constructing a new algorithm.

- (ii) CTOUGH contains many lines of code that are not needed by **MULTIFLO** which pertain to its use in modeling geothermal energy reservoirs. This added code consumes valuable memory resources and may slow computation time.
- (iii) CTOUGH is a vectorized code and as such is difficult to modify.
- (iv) CTOUGH incorporates boundary conditions in a computationally extremely inefficient manner by including the boundary nodes in the computational domain, thus increasing the size of the jacobian matrix and cpu time.
- (v) The air mass fraction does not appear to be calculated by CTOUGH with sufficient accuracy necessary to estimate air concentrations at the *ppb* level.
- (vi) Several problems appear to exist extending CTOUGH to very high temperatures ( $\sim 1600^{\circ}\text{C}$ ) needed to model moisture redistribution around dikes and volcanoes.
- (vii) The experience gained from modifying and improving the computational efficiency of CTOUGH can be directly incorporated into the new algorithm.

A sequentially coupled methodology is envisioned to solve the multidimensional, multiphase, multicomponent fluid and solute flow and transport equations in a partially saturated porous medium. In this approach heat and solvent mass conservation equations are solved separately from solute mass conservation equations. Thus at each new time step, first the heat and mass flow equations are solved simultaneously to obtain the temperature, pressure, saturation and flow field as functions of distance. Second, chemically reacting solutes are transported using the results obtained from solving the heat and solvent mass conservation equations. As a third step, mineral concentrations are calculated enabling changes in porosity, tortuosity and permeability to be computed which can then alter the flow field. This three-step approach can be justified based on the different time scales of the processes involved. Thus alteration of rock properties through chemical reactions proceeds much more slowly compared to changes in the aqueous solution composition and flow and temperature fields caused by decay of the radioactive waste form. Another way to put it, the system adjusts quasi-statically to chemical alteration of the host rock.

This is expected to be a good approximation for sufficiently dilute solutions in which density corrections are not important. In the future it may prove necessary to extend the model to fully couple the solvent and solute flow and transport equations.

The time-stepping algorithm to be used will involve different strategies depending on the dimensionality of the problem. For 1D systems a fully implicit time-stepping algorithm with dynamically computed adaptive time steps will be used to solve both the heat and solvent transport equations and the geochemical reactive transport equations. For 2D problems an operator splitting algorithm will be employed in which flow and transport time steps will be decoupled from the chemical algorithm.

Initially the code will be applied to a 1D problem for a repository-scale model incorporating a heat source derived from the decay of radionuclides. This problem is similar to that investigated by Lichtner and Walton (1994), but will also include chemical reaction of the tuffaceous host rock and changes in solution composition resulting from evaporation and condensation.

## 2.4. Data Flow and User Interface

A flow chart illustrating the general structure of the code **MULTIFLO** is presented in Figure 1. **MULTIFLO** will be structured to allow each basic process: fluid flow, heat flow and transport,

two-phase flow, and reactive transport to be run in combination or individually. The possible combinations of processes are listed in Table 1 indicating a maximum of 9 relevant possibilities. This structure will facilitate individual testing of the modules and benchmarking them against existing codes such as CTOUGH and PORFLO. Each flow or transport process consists of five basic subroutines with the functions of initialization, time-integration, field variable updating, time-step control, and testing.

The code is run on a UNIX system by entering the command:

```
multiflo [-i] input -o output -d database ...
```

where the square brackets designate that `-i` need not be entered in the command line, `input` represents the input file, `output` the output file, and `...` stands for possible additional options to be specified at a later date.

Table 1: Processes-icode parameter.

icode	single process	icode	multiple processes
1	fluid flow	4	heat flow + fluid flow
2	gem (reactive transport)	5	two-phase flow
3	heat flow	6	fluid flow + gem
		7	heat flow + gem
		8	heat flow + fluid flow + gem
		9	two-phase flow + gem

#### 2.4.1. Initial and Boundary Conditions

In order to avoid numerical difficulties at early times, it is necessary to use a flux boundary condition for the two-phase flow module. Otherwise the initial infiltration rate becomes extremely large approaching infinity as the time step approaches zero. This causes numerical oscillation in the transport module due to the Peclet number approaching infinity.

#### 2.4.2. I/O

Input data necessary for defining a run is read from a free-format input file. Auxiliary input files include a geochemical database that may be specified by the user. The default geochemical database is equivalent to the EQ3/6 database, modified to reflect recent changes in thermodynamic data available from the literature.

Output is written to specified data files in the form of a spreadsheet-like format that can be easily read from a stand-alone graphics application for plotting. A log file will record the time and date of the run, echo the input file, and record various results of the initialization routines such as the aqueous solution composition of the initial and infiltrating fluid if relevant.

#### 2.5. Hardware and Software Requirements

The code **MULTIFLO** will be written in ANSI FORTRAN 77 extended to allow for the use of `do-enddo` and `include` statements as well as system-dependent calls for timing routines. The code will run on a SUN workstation or PC platform with the appropriate FORTRAN compiler.



## 2.6. Graphics

No special graphics output devices are required. Output will be in the form of ascii files written in a spreadsheet-like format that can be read in by the user's favorite graphics software.

## 2.7. Pre- and Post-Processors

No pre- or post-processors will be needed.

## 3. REFERENCES

- Lichtner, P. C. 1994a. *Multi-Phase Reactive Transport Theory*. CNWRA 94-018. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.
- Lichtner, P. C. 1994b. *Engineered Barrier System Performance Assessment Codes (EBSPAC) Progress Report October 1, 1993, through September 25, 1994*. CNWRA 94-026. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.
- Lichtner, P. C. and Walton, J. C. 1994. *Near-Field Liquid-Vapor Transport in a Partially Saturated High-Level Nuclear Waste Repository*. CNWRA 94-022. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.
- Nitao, J. J. (1990) V-TOUGH—An enhanced version of the TOUGH code for the thermal and hydrologic simulation of large-scale problems in nuclear waste isolation. *UCID-21954*, Lawrence Livermore Laboratory, 24p.
- Pruess, K. (1987) TOUGH user's guide. Lawrence Berkeley Laboratory Report, LBL-20700.
- Walton, J. C. and Lichtner, P. C. 1995. *Quasi-Steady State Model for Coupled Liquid, Vapor, and Heat Transport: Application to the Proposed Yucca Mountain High-Level Waste Repository*. CNWRA 94-0???. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.
- Zyvoloski, G., Dash, Z., Kelkar, S. 1992 FEHMN 1.0: Finite element heat and mass transfer code. *LA-12062-MS*, Rev 1. Los Alamos, NM, Los Alamos National Laboratory.

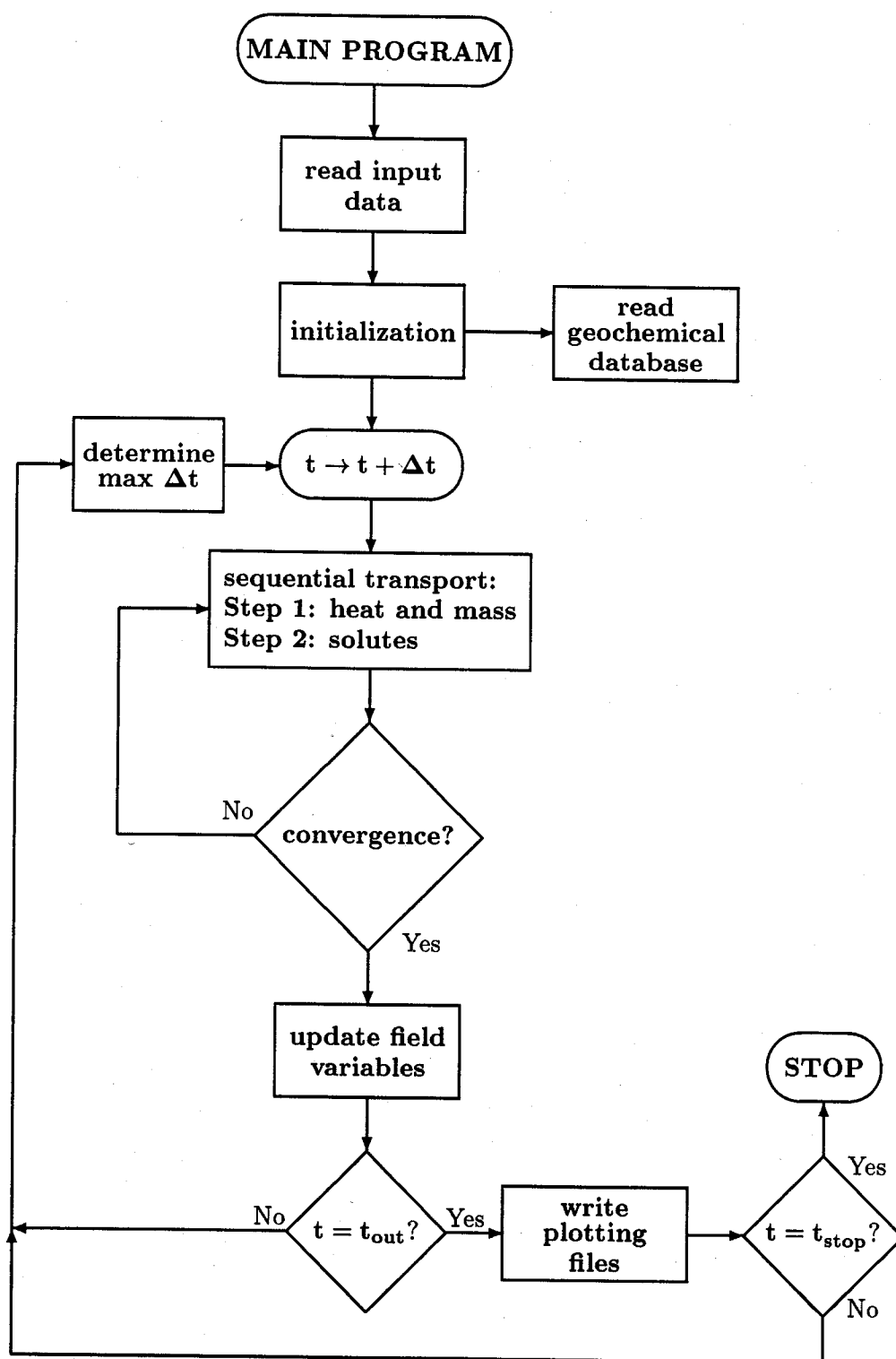


Figure 1: Flow diagram for the computer code **MULTIFLO**.