

CNWRA A center of excellence in earth sciences and engineering

A Division of Southwest Research Institute™
6220 Culebra Road • San Antonio, Texas, U.S.A. 78228-5166
(210) 522-5160 • Fax (210) 522-5155

December 13, 2001
Contract No. NRC-02-97-009
Account No. 20.01402.562

U.S. Nuclear Regulatory Commission
ATTN: Dr. John W. Bradbury
Division of Waste Management
Two White Flint North, Mail Stop TD-13
Washington, DC 20555

SUBJECT: Transmittal of the deliverable "MULTIFLO Version 1.5 User Guide Update"
(IM 01402.562.210).

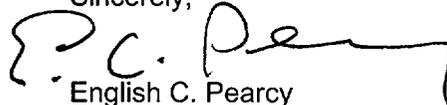
Dear Dr. Bradbury:

This letter transmits the deliverable "MULTIFLO Version 1.5 User Guide Update" (IM 01402.562.210). This user guide is intended to provide additional assistance using the previously released Version 1.5 of the MULTIFLO code. Version 1.5 includes specific features important to evaluating repository performance, including a free-drainage boundary condition, and an improved description of fracture-to-matrix flow.

The MULTIFLO code continues to be the main tool for U.S. Nuclear Regulatory Commission process-level modeling of coupled mechanisms important to repository performance. Rigorous testing and benchmarking activities have produced major improvements in accuracy and reliability. MULTIFLO is now used to conduct detailed process-level analyses for several key technical issues. These analyses support development of abstractions for performance assessment calculations and are used to evaluate U.S. Department of Energy work related to agreement items resulting from the key technical issue meetings over the last year.

If you have any questions about this deliverable, please contact me 210.522.5540 or Dr. Scott Painter 210.522.3348.

Sincerely,



English C. Pearcy
Element Manager
Geohydrology and Geochemistry

s:\phouston\MULTIFLO user guide letter.wpd
Enclosure

cc:	J. Linehan	W. Reamer	S. Painter	W. Patrick
	D. DeMarco	K. Stablein	R. Pabalan	B. Sagar
	E. Whitt	D. Esh	L. Browning	CNWRA Directors w/o enclosure
	B. Meehan	R. Codell	G. Ofoegbu	CNWRA Element Mgrs w/o enclosure
	J. Greeves	T. McCartin	R. Green	T. Nagy (SwRI Contracts)
	D. Brooks	H. Arlt	M. Hill	P. Maldonado
	J. Piccone			M. Seth
	B. Leslie			



Washington Office • Twinbrook Metro Plaza #210
12300 Twinbrook Parkway • Rockville, Maryland 20852-1606

**MULTIFLO USER'S MANUAL
TWO-PHASE NONISOTHERMAL COUPLED
THERMAL-HYDROLOGIC-CHEMICAL
FLOW SIMULATOR**

MULTIFLO VERSION 1.5

Prepared for

**Nuclear Regulatory Commission
Contract NRC-02-97-009**

Prepared by

**Mohan S. Seth
Technical Software and Engineering
Richardson, Texas**

**Scott Painter
Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas**

**Revision 3
Change 0**

December 2001

CONTENTS

Section	Page
FIGURES	vi
TABLES	vii
ACKNOWLEDGMENTS	viii
1 INTRODUCTION	1-1
1.1 Overview of METRA	1-2
1.2 Overview of GEM	1-4
1.3 The MULTIFLO Driver	1-5
1.4 Hardware and Software Requirements	1-6
2 INPUT DATA	2-1
2.1 Input Data Structure	2-1
2.1.1 Keywords	2-1
2.1.2 Comment Lines	2-1
2.1.3 SKIP/NOSKIP Keywords	2-1
2.2 METRA Input Data Keywords	2-2
2.2.1 Fixed Data	2-3
2.2.1.1 Title Lines	2-3
2.2.1.2 Run-Type Keyword	2-3
2.2.2 Initialization Data Keywords	2-4
2.2.2.1 Pressure-Volume-Temperature Properties of Component 2 [CMP2]	2-7
2.2.2.2 Pure Heat Conduction [CONduction]	2-8
2.2.2.3 Node Connections [CONNECTIONS]	2-9
2.2.2.4 Grid-Block Coordinates [CXYZ]	2-11
2.2.2.5 Dual Continuum Model Parameters [DCMPParameters] ..	2-14
2.2.2.6 Depths of Grid Blocks [DEPTH]	2-15
2.2.2.7 Grid-Block Sizes [DXYZ]	2-17
2.2.2.8 Equilibration [EQUilibration]	2-19
2.2.2.9 Grid Geometry [GRID]	2-21
2.2.2.10 Initial Condition [INIT]	2-23
2.2.2.11 Klinkenberg Gas Slippage Parameters [KLINKenberg] ...	2-25
2.2.2.12 Single-Phase Liquid System [LIQUid]	2-27
2.2.2.13 Multiple Interacting Continua [MINC]	2-28
2.2.2.14 Rock Saturation Characteristic Properties [Pckr]	2-29
2.2.2.15 Rock Properties [PHIK]	2-34
2.2.2.16 Rock Thermal Properties And Binary Diffusion Data [THERmal]	2-39
2.2.3 Recurrent Data Keywords	2-41
2.2.3.1 Automatic Time Step Control Data [AUTOSTep]	2-42

CONTENTS (continued)

Section		Page
	2.2.3.2	Boundary Condition Data [BCON] 2-44
	2.2.3.3	Maximum Time Step Limit [LIMIt] 2-48
	2.2.3.4	Output [OUTPut] 2-50
	2.2.3.5	Plotting Results [PLOTs] 2-52
	2.2.3.6	Beginning of Recurrent Data [RECUrrent] 2-53
	2.2.3.7	Solution Method [SOLVe] 2-54
	2.2.3.8	Source/Sink [SOURce] 2-56
	2.2.3.9	Steady State [STEAdy] 2-59
	2.2.3.10	Target Times [TIME] 2-60
	2.2.3.11	Convergence Tolerances [TOLR] 2-62
	2.2.4	Auxiliary Keywords 2-63
	2.2.4.1	Debug Output For Initialization [DEBUg] 2-64
	2.2.4.2	Run Terminator [ENDS] 2-66
	2.2.4.3	Monitoring Nodes [MONItor] 2-67
	2.2.4.4	Restart Options [RSTArt] 2-68
2.3	GEM Input Data Keywords 2-69	
	2.3.1	Title Lines 2-69
	2.3.2	Input Data Keywords 2-69
	2.3.2.1	Aqueous Secondary Species [AQCX] 2-71
	2.3.2.2	Kinetic (Irreversible) Homogeneous Aqueous Reactions [AQIR] 2-73
	2.3.2.3	Boundary Conditions [BCON] 2-75
	2.3.2.4	Break-Through Node Points for Plotting [BRKP] 2-79
	2.3.2.5	Initial Conditions and Definition of Component Species [COMPOnents] 2-80
	2.3.2.6	Option for Computing Conserved Quantities [CONSeRve] 2-84
	2.3.2.7	Coupling METRA and GEM [COUPlE] 2-85
	2.3.2.8	Thermodynamic Database File [DBASe] 2-87
	2.3.2.9	Dual Continuum Model Parameters [DCMParameters] . . 2-88
	2.3.2.10	Aqueous and Gaseous Diffusion [DIFF] 2-90
	2.3.2.11	Initial and Maximum Time Step [DTSTep] 2-92
	2.3.2.12	Grid-Block Sizes [DXYZ] 2-94
	2.3.2.13	End of Run [ENDS] 2-96
	2.3.2.14	Liquid and Gas Flow Velocities and Dispersivity [FLOW] 2-97
	2.3.2.15	Gaseous Species [GASeS] 2-98
	2.3.2.16	Grid Geometry [GRID] 2-99
	2.3.2.17	Ion-Exchange Reactions [IONX] 2-101
	2.3.2.18	System Parameters [ISYSem] 2-102
	2.3.2.19	Setting Master Species For Time Step Control [MASTer] 2-104
	2.3.2.20	Kinetic (Irreversible) Mineral Reactions [MNIR] 2-105
	2.3.2.21	Mineral Species [MNRL] 2-108
	2.3.2.22	Various Parameters and Options [OPTS] 2-109
	2.3.2.23	Writing Plot Files [PLTFiles] 2-112

CONTENTS (continued)

Section		Page
	2.3.2.24 Initial Temperature and Pressure [PTINit]	2-114
	2.3.2.25 Method of Solution [SOLVe]	2-115
	2.3.2.26 Source/Sink [SOURce]	2-117
	2.3.2.27 Relative Tolerances [STOL]	2-120
	2.3.2.28 Target Time [TIME]	2-121
	2.3.2.29 Convergence Tolerances [TOLR]	2-122
	2.3.2.30 Node Volume [VOLUme]	2-123
3	SAMPLE INPUT DATA	3-1
3.1	METRA Input File	3-1
3.1.1	METRA Sample Input File: Two-Dimensional Radial Geometry	3-1
3.2	GEM Sample Input Data: Two-Dimensional Repository Problem	3-5
4	EXPLANATION OF OUTPUT RESULTS	4-1
4.1	Screen Display	4-1
4.1.1	METRA Screen Display	4-2
4.1.2	Screen Display	4-3
4.1.3	MULTIFLO Screen Display	4-5
4.2	METRA Output	4-7
4.2.1	Initialization Output	4-7
4.2.1.1	Mass and Energy in Place	4-7
4.2.1.2	Initial Conditions	4-8
4.2.1.3	Transmissibility	4-9
4.2.1.4	Binary-Diffusion Transmissibility	4-10
4.2.2	Recurrent Output	4-10
4.2.2.1	Mass and Energy in Place	4-10
4.2.2.2	Inner Iteration Counter	4-10
4.2.2.3	Err-H ₂ O, Err-Air, Err-Eng	4-11
4.2.2.4	ICONV	4-11
4.2.2.5	DPMAX, DSMAX, and DTMPMX	4-12
4.2.2.6	Balances	4-12
4.2.2.7	Boundary Condition Influx Summary	4-12
4.2.2.8	Source/Sink Summary	4-12
4.2.2.9	Velocities	4-12
4.2.2.10	Plot Files	4-13
4.2.2.11	Other Files	4-13
4.3	GEM Output	4-13
5	INSTALLATION AND EXECUTION	5-1
5.1	Installation	5-1
5.2	Execution of MULTIFLO, GEM, and METRA	5-2

CONTENTS (continued)

Section		Page
	5.2.1 MULTIFLO	5-2
	5.2.2 GEM	5-2
	5.2.3 METRA	5-3
5.3	Redimensioning	5-3
5.4	Machine Specific Routines	5-5
5.5	Compilation	5-5
6	REFERENCES	6-1
APPENDIX A		
APPENDIX B		

FIGURES

Figure		Page
2-1	Coordinate Systems Used for Cartesian and Radial Geometries	2-11
2-2	Boundaries of Computational Domain in Cartesian Coordinates	2-45

TABLES

Table		Page
1-1	Choice of Primary Variable for Different Fluid States	1-3
2-1	METRA Keywords	2-5
4-1	List of Time-History Plot Files and Associated Variables	4-13
4-2	List of METRA Plot Files Printed at Target Times and Associated Variables for Plotting Spatial Data	4-14
4-3	Unit Numbers and Associated Files	4-14
4-4	List of Plot Files Containing Spatial Profile Data at Times Specified on the Time Keyword	4-15
4-5	List of Plot Files Containing Time-History Data at Spatial Nodes Specified on the BRKP Keyword	4-15

ACKNOWLEDGMENTS

This guide was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the U.S. Nuclear Regulatory Commission (NRC) under Contract No. NRC-02-97-009. The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards Division of Waste Management. The report is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC. Sources of data are referenced in each chapter. The respective sources of these data should be consulted for determining their levels of quality assurance.

The original version of this document was principally authored by Dr. Peter Lichtner, as were the early versions of the MULTIFLO code. The authors of this revision gratefully acknowledge Dr. Lichtner's contributions. The authors also acknowledge the technical reviews of James R. Winterle and Goodluck Ofoegbu, the programmatic review of Budhi Sagar, and the editorial review of Barbara Long. Special appreciation is due to Paulette Houston and Arturo Ramos for their tireless assistance in the preparation of the manual.

QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: CNWRA-generated original data contained in this report meets quality assurance requirements described in the CNWRA Quality Assurance Manual. Sources for other data should be consulted for determining the level of quality for those data.

ANALYSES AND CODES: This computer code has been developed under the CNWRA Software Configuration Procedures. This controlled MULTIFLO Version 1.5 replaces Version 1.2.3, which was released December 2000.

1 INTRODUCTION

The computer code MULTIFLO was developed to aid in understanding perturbations to the near-field environment surrounding a high-level nuclear waste underground disposal facility following emplacement of the waste. The computer code MULTIFLO describes coupled thermal-hydrological-chemical processes in one-, two-, and three-dimensional spatial dimensions. MULTIFLO is a general code for simulating multiphase, multicomponent transport processes in nonisothermal systems with chemical reactions and reversible and irreversible phase changes in solids, liquids, and gases. The proposed high-level waste disposal site at Yucca Mountain, Nevada, is unique in that the site lies above the water table. This circumstance has profound consequences on the behavior of the near-field environment surrounding the repository in response to heat generated by the radioactive waste. Perturbations to the near-field environment caused by emplacement of the waste consist primarily of (i) changes in temperature, pressure, and moisture distribution; (ii) modification of gaseous and aqueous flow fields including the formation of heat pipes; (iii) changes in composition of aqueous and gaseous phases; and (iv) alteration of the host rock resulting in changes in porosity, permeability, tortuosity, and sorptive properties. Important aqueous and gaseous solution variables that influence degradation of the waste package and spent fuel and radionuclide transport, include the pH, chloride concentration, and oxygen and carbon dioxide fugacities. Alteration of cristobalite in the Yucca Mountain tuffaceous host rock to quartz may result in an increase in porosity and permeability in the near field. The computer code MULTIFLO was developed in an effort to model and understand the evolution of the near-field environment surrounding a high-level waste repository emplaced in a partially saturated host rock.

The code MULTIFLO consists of two sequentially coupled submodules: Mass and Energy TRANsport (METRA) and General Electrochemical Migration (GEM). METRA solves mass balance equations for water and air and an energy balance equation. The submodule GEM solves mass balance equations for multicomponent reactive transport of solute species. GEM takes into account aqueous speciation of solutes, gaseous speciation, mineral precipitation and dissolution reactions, and ion-exchange, and sorption. GEM uses the flow field, temperature, pressure, and saturation state computed by the METRA submodule for computing reactive transport of aqueous and gaseous species. The flow field computed by METRA can be altered through changes in porosity and permeability computed from GEM. Both METRA and GEM can also be run in stand-alone mode.

This user's manual replaces and supersedes the users manual for MULTIFLO 1.2, which was released in February, 2000. The revisions to the user's manual document changes to the input format associated with code changes and additional capabilities introduced in the move from version 1.2.3 to version 1.5. In particular, a new gravity drainage boundary condition was introduced for METRA, and the high-resolution spatial differencing schemes in GEM were extended to three-dimensional. In addition, several coding errors and errors in the manual were uncovered and corrected as part of the ongoing testing process.

This user's manual is intended primarily to provide information and instructions to users in the preparation of input data. In addition to a detailed description of input data format and

structure, an overview of the general capabilities and limitations of the code, explanation of various output results, procedure for compilation and run execution, and the other user-oriented features are provided. Appendixes are provided that give a brief outline of the mathematical equations on which METRA and GEM are based. A more detailed development and discussion of the mathematical basis for the partial differential equations solved by the code MULTIFLO with several examples may be found in Lichtner (1996). In this manual, all computer input, screen output, filename and executables appear in Courier font.

1.1 Overview of METRA

METRA is a two-phase, three-dimensional nonisothermal flow code. Simulation of simpler systems are also possible for zero, one, or two spatial dimensions with a single- (all liquid or gas) or two-phase fluid. Rock with zero porosity allows simulation of pure heat conduction problems. The equation of state for pure water allows temperature ranges of 1–800 °C and pressures below 165 bars. METRA is based on a fully implicit formulation using a variable substitution approach. Space discretization is based on a block-centered grid employing an integral finite-volume difference scheme suitable for unstructured grid with arbitrary interblock grid connectivity and any polygonal block boundary. For ease of input, data preparation, and to retain compatibility with the preceding MULTIFLO Version 1.0, a preprocessor is incorporated that converts the Cartesian, and cylindrical geometries and couches the data in a format required for the general unstructured grid. Flow in fractured media may be represented by the dual continuum model in addition to the equivalent continuum model formulation where a dual continuum is represented by an equivalent single continuum. The multiple interacting continuum model is not included in the version, but can be implemented by defining an unstructured grid in the appropriate way. For a two-phase nonisothermal system consisting of two species, water and air, a minimum of three primary variables is required to describe the system. The primary variables chosen are listed in Table 1-1, in which p_l is the liquid pressure for a pure liquid system and p_g total gas pressure for a two-phase or pure gas-phase system. The mole fraction of air is denoted by X_a , with partial pressure p_a , s_g denotes gas saturation, and T denotes the temperature.

The three primary equations solved by METRA are (i) total mass balance, (ii) air mass balance, and (iii) energy balance. The three equations for each grid block are solved simultaneously using the block tri-diagonal Thomas algorithm (for one-dimensional problems) and, optionally, by the WATSOLV package (van der Kwaak, et al., 1995). The WATSOLV package is based on incomplete factorization (ILU) followed by acceleration employing generalized minimum residual (GMRES) (van der Kwaak, et al., 1995) or biconjugate gradient stabilized (CGSTAB) (van der Kwaak, et al., 1995) procedures. This package is suitable for both two- and three-dimensional problems.

The code METRA treats mass transport by (i) Darcy's law (as modified by the relative permeability for multiphase flow), which includes capillarity, gravity, and viscous forces; and (ii) diffusion of air-vapor. Energy transfer is treated for convective and conductive processes. Arbitrary user-specified spatial variation in porosity, absolute rock permeability (in all three spatial directions), rock tortuosity, thermal conductivity, rock characteristic curves (relative permeability and capillary pressure), and other pertinent factors are included in the code.

Table 1-1. Choice of Primary Variable for Different Fluid States	
Fluid State	Primary Variables
Single-phase liquid	ρ_l, X_a, T
Two-phase	ρ_g, ρ_a, S_g
Single-phase gas	ρ_g, ρ_a, T

In addition to Cartesian or cylindrical geometries, other coordinates may be readily treated by directly reading the input data in an unstructured grid format. Vapor-liquid equilibria may be defined with lowered vapor pressure resulting from capillary forces. Efforts were made to design the code efficiently from computational as well as memory considerations. It is expected that with 128 MB memory, three-dimensional two-phase problems with over 50,000 grid blocks can be accommodated. For single-phase flow or heat conduction only, over 100,000 grid blocks should be easily accommodated. Time-dependent boundary conditions are accommodated in the code and include both Dirichlet (constant field variables) and Neumann (constant flux) types. Heat transfer by radiation at the boundary is also considered. The boundary conditions can be specified as a function of time. Heat and mass sources and sinks may be designated at desired grid nodes and varying with time. Time dependent boundary conditions and source/sink are specified in tabular form which are linearly interpolated corresponding to the midpoint of the time step.

Some of the other features included in the simulator are as follows. Flexible output can be obtained at specified times or time steps. Output also includes data files for graphical post processing and restart files. Intermediate variables may be printed by debug options. Mass transfer in the gas phase includes enhanced binary diffusion. Extensive default parameters are provided for properties of air, convergence criteria, method of solution, diffusion parameters, and a host of others. Pressure-volume-temperature properties for H₂O are calculated optionally by a rapid table look-up procedure or by using the International Formulation Committee (1967) functions. Gas mixture properties are calculated assuming the ideal gas law. Gas viscosity is computed using the kinetic theory of gases (Hirschfelder, et al., 1954). Arbitrary general heterogeneity for all rock parameters including capillary pressure and relative permeability curves is possible. Options are available for van Genuchten, linear, tabular, and Corey's Equations for saturation-dependent properties. Rocks with matrix and fractures may be modeled in one of the following two manners:

- Equivalent continuum model in which it is assumed that the capillary pressure for the matrix equals that of fractures
- Dual continuum model approach where the matrix and fracture constitute two discrete continua and are represented by two (overlapping) grid blocks at each node in space

An alternative approach to modeling fractured rock flow and transport, the multiple interacting continuum representation, is not implemented directly in this version. However, the multiple interacting continuum representation may be implemented by using the unstructured grid option

with appropriately defined connections between nodes. In the multiple interacting continuum representation each matrix block is partitioned into an arbitrary chosen number of concentric parallelepipeds where the outermost portion connects with the fracture allowing for gradients within the matrix. Flow from (into) matrix to (from) fracture is assumed to be one-dimensional with no effect of gravity within the matrix block. Unlike the dual continuum model, matrix blocks are not connected with each other but communicate only through the fracture.

Vapor pressure lowering of H₂O-phase behavior optionally accounts for the lowered vapor pressure because of capillary pressure as defined by Kelvin's equation. Options exist for automatic time-step-size calculation, and provision to cut a time step repeatedly to ensure the solution vector changes within a specified limit. In the event the solution fails to converge within a maximum of 25 time step cuts, the program will stop with an appropriate message.

Partial dynamic memory management based on run time parameters has been implemented in the code. Mass and energy balances are calculated based on cumulative and incremental balances to monitor the accuracy of the solution.

1.2 Overview of GEM

The code GEM solves multicomponent-multiphase, nonisothermal, reactive mass transport equations for one-, two-, or three-dimensional problems. Simultaneous transport in both liquid and gas phases is possible. Transport in a pure gas phase is not currently implemented. Both advective and diffusive transport are incorporated in the code. Chemical reactions consist of homogeneous aqueous reactions in local chemical equilibrium, redox reactions, mineral precipitation and dissolution reactions treated kinetically, and ion-exchange reactions. In stand-alone mode, GEM may use a constant flow velocity read from an input file or a steady-state flow field provided by the user. In addition, a prescribed saturation field may be read in. One-way coupling to METRA allows the transient flow field computed from METRA to be sequentially fed into GEM. Two-way coupling is also possible in which changes in porosity and permeability resulting from mineral precipitation and dissolution may be fed back to METRA from GEM. The code applies generally to heterogeneous porous media.

A number of solution algorithms are available in GEM including implicit, explicit, and operator-splitting finite difference methods. Solvers available include a tri-diagonal solver and the conjugate gradient solver WATSOLV (van der Kwaak, et al., 1995). The implicit finite difference algorithm for solving reactive transport equations is generally only suitable for one-dimensional problems or small two-dimensional problems because of the prohibitive memory requirements for large two-dimensional problems. The operator-splitting algorithm, in which the solution algorithm is broken down into a nonreactive followed by a reactive time step, is recommended for large two- and three-dimensional problems. Transport in the operator-splitting algorithm may be treated implicitly or explicitly. The explicit finite difference scheme is also applicable to large problems. Four variants of the Total Variation Diminishing algorithm are available for high Peclet number flows.

Two thermodynamic databases are provided with GEM: (i) `master25.V8.R6` and (ii) `mastertemp.V8.R6`. Both databases are derived from the EQ3/6 database

(Wolery, 1983). The first file (`master25.V8.R6`) contains equilibrium constants at 25 °C only, whereas the second file (`mastertemp.V8.R6`) contains equilibrium constants over the temperature range from 0–300 °C. These are stored at temperatures of 0, 25, 60, 100, 150, 200, 250, and 300 °C along the saturation curve of water and interpolated at intermediate values using a Mayer-Kelly function given in Appendix B [Eq. (B-21)].

One limitation of the current version of GEM is that it cannot handle a pure gas phase system or a spatial region in which only a single gas phase is present. Some amount of liquid must always be present. This is because the chemistry in GEM is defined through a set of primary species that belong to the aqueous phase. In the presence of a pure gas phase region, it would be necessary to use primary species from the gas phase only. At the interface between a pure liquid or two-phase region and a pure gas phase region, different sets of primary species are necessary to describe the chemical reactions in the system. At present, employing different sets of primary species in different regions of space is not possible. To handle situations with a pure gas phase a saturation cutoff specified by the user is introduced in those regions.

1.3 The MULTIFLO Driver

The MULTIFLO driver program controls the interaction of the submodules METRA and GEM. The code MULTIFLO is designed so that the submodules METRA and GEM may be run individually in stand-alone mode without coupling to one another, in which case, both codes have their own main driver programs. They may also be run from the MULTIFLO driver program in stand-alone or coupled mode by appropriately setting the parameter `icode`. There are four possible choices for `icode`:

- `icode = 1`, METRA stand-alone
- `icode = 2`, GEM stand-alone
- `icode = 3`, Coupled METRA and GEM in transient mode
- `icode = 4`, Coupled METRA and GEM with steady-state flow field and GEM in transient model

The parameter `icode` is entered following a prompt from MULTIFLO:

```
- read icode: (1-metra, 2-gem, 3-coupled, 4-coupled: steady-state)
```

With `icode = 1` and `2`, METRA and GEM are run in stand-alone mode. For `icode = 3` and `4`, METRA and GEM are coupled through the MULTIFLO driver. For `icode = 3`, GEM is called after each successfully completed METRA time step. For `icode = 4`, first METRA is run until a steady-state solution is obtained, and then GEM is called using the steady-state METRA solution. In coupled mode (`icode = 3` and `4`), the target time for writing plot files is taken from the GEM input file, whereas the grid spacing, porosity, temperature, pressure, and saturation are taken from the METRA input file.

1.4 Hardware and Software Requirements

The MULTIFLO code is written in the ANSI FORTRAN 77 programming language. The code was developed and tested on a SUN workstation and a PC running Windows NT. It can also be run under HP workstations, and on a PC with the DOS operating system using the Lahey-Fortran compiler. Version 1.5 of MULTIFLO contains approximately 80,000 lines of code including comment lines. The GEM submodule consists of approximately 20,000 lines of code and the METRA submodule consists of approximately 15,000 lines of code not including comment lines. The complete source code occupies 2.3 MB of disk space uncompiled and 13.5 MB compiled, with full optimization on a SUN workstation, including the three executable files `multiflo`, `metra`, and `gem`. The size of executable modules will vary with compiler options.

The amount of RAM required to run the code depends on the size and complexity of the problem considered. For large problems or if only relatively small problems are run, the user may easily tailor various array dimensions to the specific demands required. On completion of these changes it is necessary, of course, to recompile the code. Make files are provided which automate this task.

2 INPUT DATA

2.1 Input Data Structure

2.1.1 Keywords

All keywords are followed by either none, one, or more set(s) of data lines depending on the type of data. A keyword can be up to 20 characters long; however, only the first four characters are used for data identification purposes, and can start anywhere on a line (the keyword does not have to start from column 1) *except* that there should be no other nonblank characters before the keyword on a keyword line. A keyword may be followed by one or more variables as dictated by the input requirements. Keywords may be in upper case, lower case, or a combination of upper and lower case letters, but must NOT have any embedded blanks. For example, the keyword THERMAL DATA is inadmissible, but THERMAL-DATA or Thermal-Data is acceptable.

2.1.2 Comment Lines

The code provides the ability to include comment lines in the input file which are ignored during processing. Comment lines are identified by a colon (:). The colon and the following text/data contained on a single line are not processed by the code. The colon can also follow data appearing on a line, in which case the information after and including the colon will be ignored. To deactivate trailing data on a line or to introduce some comment on a data line, an exclamation mark (!), in place of a colon, may also be introduced such that all information on a data line after and including the exclamation mark is ignored.

2.1.3 SKIP/NOSKIP Keywords

A facility is provided to skip over one or more segments of data in the input file without physically deleting these lines of data. This procedure is invoked by means of the SKIP and NOSKIP keywords.

Read: ISKIP

ISKIP Keyword to mark beginning and end of skipped data.

- = SKIP marks the beginning of data to be skipped. Input data are skipped and are not to be processed following this line until a NOSKIP keyword is encountered.
- = NOSKIP marks the end of the input data to be skipped. All data following this keyword are processed until a new SKIP keyword is encountered. This keyword has no effect if a SKIP keyword is not introduced prior to the NOSKIP keyword. In effect, the keyword NOSKIP negates the effect of the SKIP keyword.

Comment(s):

If a segment or block(s) of data is not to be processed, insert a SKIP keyword at the beginning of such a block and enter a NOSKIP keyword at the end of the block. Repeated use of SKIP and NOSKIP keywords has the effect of removing the data between the SKIP and NOSKIP keywords in the data file during execution while preserving the entire input data file intact. If a NOSKIP keyword is not encountered following a SKIP keyword, all data following the SKIP keyword will be ignored. If the NOSKIP keyword is not preceded by the SKIP keyword, it will have no effect, and will be ignored.

Example:

|
Data

|
SKIP: Ignore data beginning with the SKIP keyword until the NOSKIP
keyword is encountered.

|
Data

|
NOSKIP Process data following the NOSKIP keyword until another SKIP
keyword is encountered.

|
Data

|
SKIP

2.2 METRA Input Data Keywords

All input data are grouped into three types:

1. Fixed Data: Two title lines and a line indicating restart or initial run. A restart run is one that is resumed from an earlier run obtained from a saved restart file.
2. Initialization Data: Time-independent data specifying material properties and initial conditions. Initialization data constitute the bulk of the input data in most cases.
3. Recurrent Data: Time-dependent data including source/sink tables, method of solution, output frequency, restart file writing, boundary conditions, tolerances, iterations, time-step sizes, target time, and such other parameters. All data in this group may be modified in subsequent time intervals.

All data are in free-format and associated with a keyword. Thus, the order of input in any particular group is generally immaterial except for the fixed data which must start with two title lines followed by the RSTART keyword. The data associated with the keyword GRID, must be the first keyword in the initialization data.

The input data must be in the order of 1. Fixed Data, 2. Initialization Data, and 3. Recurrent Data. If only Initialization is to be carried out, the run can be stopped without marching in time with a run terminator keyword ENDS after the Initialization Data.

The record length for free-format input data file must not exceed 256 characters. The free-format allows variables to be read in without regard to field boundaries except that they are separated by one or more contiguous spaces or a comma (,) or a combination of them. Successive appearance of the same value for variables may be represented by $n*x$, where n is the successive appearance of variables all of which have a common value x . Unlike standard Fortran, a character string (alphanumerics) does not have to be and should not be enclosed in apostrophes or quotation marks. Likewise trailing zeros may be left as blanks on a line. A carriage return is treated like a blank. Two consecutive commas will mean a null value for the corresponding variable.

In the following examples, the input data given by (a), (b), and (c) are equivalent.

```

1 -101, 5. 5.e0 5.0 3. 2. .2e+1 2. 2.0 7           (a)
1 -101, 3*5. 3.0, 4*2. 7                           (b)
1 -101 3*5. 3.0 4*2.e0 7                             (c)

```

The actual number of input-data records associated with certain keywords is arbitrary. In such cases, a terminator signaling the end of data for a given keyword must be entered as the last line following all the required data for the keyword. The METRA code uses a single character slash (/), asterisk (*), or period (.) in column 1 as the terminator. A blank may not be used as terminator as blank line in the input file is ignored.

2.2.1 Fixed Data

2.2.1.1 Title Lines

Two title lines are required, and these must be the first two lines in a data file. Any alphanumeric characters may be assigned for the title with up to 80 characters per line. If no title or only a one-line title is desired, simply read a blank line(s) to fulfill the two-line requirement. Comment lines beginning with a ':' (colon), and SKIP/NOSKIP can precede the title data.

The title lines should precede the run-type keyword as below.

2.2.1.2 Run-Type Keyword

The run-type keyword identifies whether a run is a normal run or a restart run. A normal run starts from time = 0, whereas, a restart run starts from time > 0.

Read: RSTART NRST

RSTART Keyword defining run type.

NRST Number of restart records from which the run is to be resumed. During a normal run (run starting from time = 0), a set of restart records may have been written at

different times. NRST specifies the particular set of records from which to resume a run. For a normal run, read NRST as zero, or simply leave the field blank.

Example: Fixed Data

```
This is a test run for a 3D dual continuum system
  April 10, 1998
:
RSTART 0 :normal run

RSTART 6 :restart run starting after the sixth restart data set.
```

Comment(s):

Note: The text on the RSTART keyword following and including the colon is not processed and is included for convenience and clarity.

For a RSTART Run (NRST > 0), skip the Initialization Data and proceed directly to the Recurrent Data section.

2.2.2 Initialization Data Keywords

The Initialization Data constitute the bulk of the data which are specified by different keywords. The data can be entered in any order with the exception of the GRID keyword which must be first. The keywords used are listed in Table 2-1.

Since the code uses only the first four characters, the remaining characters in several of the keywords (shown in lower case) are used only for a more descriptive identification of the keyword. As mentioned before, the entire keyword may be in small case, capital, or any combination of small and capital letters. For example, CONDUCTION, conduction, Conduction, CONduction, COND, and cond are valid keywords.

The presentation in Table 2-1 is in alphabetical order, although the data may be entered in any order, except for the GRID keyword which must be at the beginning of the Initialization Data as it controls the required input data for several keywords.

Table 2-1. METRA Keywords		
Keyword	Status	Comments
Initialization Data Keywords		
CMP2	Optional	
CONduction	Conditional	
CONNections	Conditional	Required for unstructured grid
CXYZ	Conditional	
DCMParameters	Conditional	Required for dual continuum model
DEPTH	Optional	
DXYZ	Conditional	
EQUllibration	Optional	
GRID	Required	First keyword
INIT	Required	
KLINkenberg	Optional	
LIQUid	Conditional	
MINC	Conditional	
PCKR	Required	
PHIK	Required	
THERmal	Required	
Recurrent Data Keywords		
AUTO-step	Optional	
BCONDition	Conditional	
LIMIt	Optional	
SOLVe	Required	
SOURce	Conditional	

Table 2-1. METRA Keywords (continued)		
Keyword	Status	Comments
STEADy	Conditional	
TIME	Required	
OUTPut	Required	
RECUrrent	Required	
TOLR	Optional	
Auxiliary Keywords		
DEBUg	Optional	
ENDS	Required	Last Keyword
MONItor	Optional	
RSTART	Optional	

2.2.2.1 Pressure-Volume-Temperature Properties of Component 2 [CMP2]

Initialization Data

Keyword: **CMP2**Optional

This keyword overrides the internally set values for properties of air (component 2). If the second component is CO₂, nitrogen, or any other gas, or if the default properties specified for air are unsatisfactory, they may be amended by this keyword. Component 1 is always designated as H₂O.

This keyword need not be used if air is the second component and the default properties are acceptable.

Read: CMP2 FMW2 SPHTC2 EQK2

CMP2 Keyword for assigning pressure-volume-temperature properties of second component.

FMW2 Molecular weight of component 2 [g/mole] (default = 28.964 g/mole).

SPHTC2 Constant volume specific heat of component 2 [J/Kg-mole-K] (default = 21232 J/Kg-mole-K).

EQK2 Proportionality constant for Henry's Law for dissolution of component 2 in liquid water [Pa]. This parameter is assumed to be temperature-independent (default = 1.e10 Pa)

Example:

```

: cmp2      fmw2  sphtc2    eqk2
  CMP2 (CO2) 16.0  0.        1.e9

```

In this example, the default value for the specific heat will be used. Note that (CO₂) is added to the keyword for identification purposes only and is not processed internally.

2.2.2.2 Pure Heat Conduction [CONduction]

Initialization Data

Keyword: **CONduction**Conditional

CONduction keyword allows calculation of heat transfer by conduction only with zero porosity and permeability. If the rock thermal conductivities CKDRY and CKSAT read by the THERmal keyword are not equal, they are internally set such that CKSAT = CKDRY. All read-in porosity and permeability values are internally set to zero. This option cannot be invoked with dual continuum model or multiple interacting continuum formulations.

If all read-in porosity values are zero and this keyword is not invoked, the code will internally set the system for heat conduction only.

There are no associated data with this keyword.

Read: CONduction

CONduction Keyword for designating the system for conduction-only heat flow with zero porosity and permeability.

Example: CONduction

2.2.2.3 Node Connections [CONNECTIONS]

Initialization Data

Keyword: **CONNECTIONS**

Required for UNSTRUCTURED grid

CONNECTIONS keyword assigns connections between nodes, nodal distances, areas, and dip-angle between the connecting nodes. This data set should be read only if the grid geometry is declared as UNSTRUCTURED on the GRID keyword, otherwise data will be read and ignored.

Read:	CONNECTIONS
Read:	M1 M2 INC IPRM1 IPRM2 DIST1 DIST2 AREA ANGLE
CONN	Keyword for reading nodal connection data.
M1, M2	Beginning and ending connected node numbers in increments of INC.
INC	Node increment. Node M1 is connected to node M1+INC, and M1+INC is connected to node M1+2*INC, and so on. That is, in general, node M1+k*INC is connected to M1+(k+1)*INC. The node-connection sequence is continued until M1+(k+1)*INC is greater or equal to M2. Default value for INC = 1. See the example below for further clarification.
IPRM1, IPRM2	Permeability directions for a pair of connecting nodes. The permeability direction is 1, 2, and 3 corresponding to x-, y-, and z-directional permeabilities [see Eq. (4-12)]. The permeability values in x-, y-, and z-directions are read by the PHIK keyword.
DIST1, DIST2	Distances of nodes to the interface between them [m].
AREA	Interface area [m ²].
ANGLE	Angle [degrees] between horizontal plane and the line joining the node centers of blocks M1 and M2. The angle is measured clockwise with reference to the horizontal plane.

Read as many lines as necessary to define all the nodal connections, and terminate the reading sequence by reading a line with slash (/), asterisk (*), or period (.) in column 1.

Example: For nodes as numbered in the following for a structured 5 × 6 grid,

```

1 2 3 4 5
6 7 8 9 10
11 12 13 14 15
16 17 18 19 20
21 22 23 24 25
26 27 28 29 30

```

the node connection data are:

```

:      m1      m2      inc iprm1 iprm2 dist1 dist2 area angle
:  horizontal connections
1       5       1       1       1       5.    5.    3.75   0.
6       10      1       1       1       5.    5.    3.75   0.
11      15      1       1       1       5.    5.    3.75   0.
16      20      1       1       1       5.    5.    3.75   0.
21      25      1       1       1       5.    5.    3.75   0.
26      30      1       1       1       5.    5.    3.75   0.
:  vertical connections
1       26      5       3       3       10.   10.   1.     90.
2       27      5       3       3       10.   10.   1.     90
3       28      5       3       3       10.   10.   1.     90
4       29      5       3       3       10.   10.   1.     90
5       30      5       3       3       10.   50    1.     90
*

```

2.2.2.4 Grid-Block Coordinates [CXYZ]

Initialization Data

Keyword: **CXYZ**

Conditional

This keyword designates the coordinates of block boundaries with reference to an origin at the southwest corner of the top surface of block (1,1,1) such that the z-axis is positive downwards as shown in Figure 2-1 (note left-handed coordinate system for Cartesian coordinates). These coordinates are used to calculate the block sizes internally. Data corresponding to this keyword should be omitted for unstructured grid, or if the block sizes are directly specified using the keyword DXYZ. If data corresponding to both keywords DXYZ and CXYZ are specified, the last values read-in will be retained.

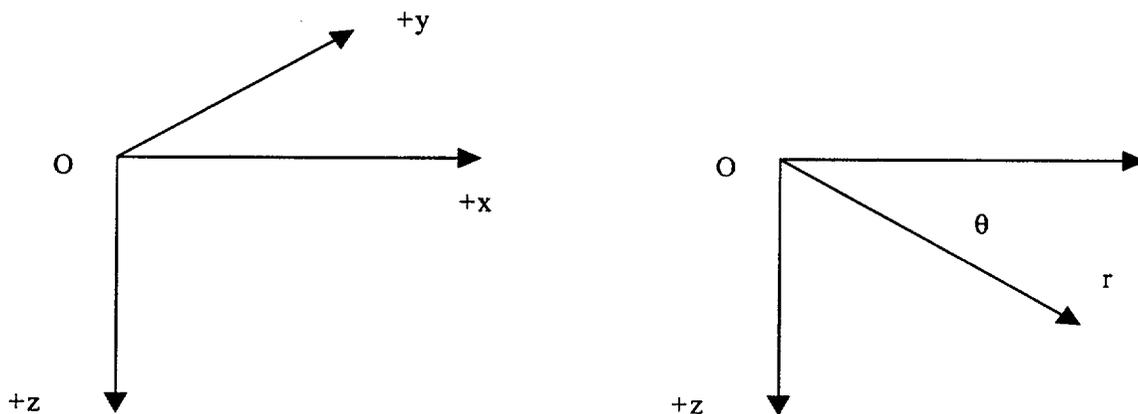


Figure 2-1. Coordinate Systems Used for Cartesian and Radial Geometries

Read: CXYZ IGRID RW RE

Read: (X(I), I = 1,NX)

Read: (Y(J), J = 1,NY)

Read: (Z(K), K = 1,NZ)

CXYZ Keyword for reading grid-block interface coordinates.

- IGRID** Index for grid-type.
- = 0 Block centered
 - = 1 Point-distributed (not implemented)
 - = 2 Boundary node at the surface corresponding to CTOUGH
- RW** Inner boundary radius for cylindrical system [m].
- RE** Outer boundary radius for cylindrical system [m].
- X** X-direction coordinates for block interfaces starting with the block interface between block 1 and 2 and ending with the outer boundary of NXth block with a total of NX values. For cylindrical system, X designates the radius to block center from the axis of the cylinder [m].
- Y** Y-direction coordinates for block interfaces in y-direction (similar to x-direction) [m]. For cylindrical systems, Y designates the angle with reference to an arbitrarily chosen zero degree plane [degrees].
- Z** Z-direction coordinates for block interfaces in the z-direction where the z-axis is positive (increases) downwards [m].

Comment(s):

Read NX values for X, NY values for Y, and NZ values for Z coordinates. If fewer than NX, NY, or NZ values are nonzero, the code will replace the zero values with the last nonzero value read.

For cylindrical geometry, if fewer than NX nonzero values are read for X coordinates, the unspecified values are computed internally based on logarithmic spacing. RW must be $<X(1)$ and $RE > X(NX)$.

For Cartesian geometry, RW and RE are not required.

Examples:

Cartesian Geometry:

```

:      igrd      rw      re
CXYZ   0         0         0

```

Cartesian Geometry:

```

:      igrd      rw      re
CXYZ  0          0      0
:x(1) x(2)...
1. 2. 3.5 5. 7. 9. 12. 15. 20. 30.! x-direction
45. 60. 100.
:y(1)
1.! y-direction
:z(1) z(2)...
10. 20. 30. 45. 60. 75. 100. 150. 12*200 !z-direction

```

This example, designates coordinates for a Cartesian grid system of 13 blocks in the x-direction, 1 block in the y-direction, and 20 blocks in the z-direction.

Cylindrical geom:

```

:      igrd rw      re
CXYZ  0      .001  100. ! radial geometry with inner and outer
                        radius of cylinder 001 and 100 m.
:
:r(1) r(2)
.5   1. 11*0.          ! only 2 values are specified.
                        The rest will be computed internally.
:
:y(1)
90.! one angular sector of 90 degrees.
:z(1) z(2) ...
10. 20. 30. 45. 60. 75. 100. 150. 12*200 ! z-direction

```

2.2.2.5 Dual Continuum Model Parameters [DCMParameters]

Initialization Data

Keyword: **DCMParameters**

Required for dual continuum model formulation

Read: DCMParameters**Unstructured Grid Read:** M1 M2 INC SIGMAF AREAMOD XLM YLM ZLM**Structured Grid Read:** I1 I2 J1 J2 K1 K2 SIGMAF AREAMOD XLM YLM ZLM

- M1, M2** Beginning and ending node numbers.
- INC** Increment of node numbers. Default value of INC = 1.
- I1, I2, J1, J2, K1, K2** Indices bounding the region in $x(r)$ -, $y(\theta)$ -, and z -directions.
- SIGMAF** Fraction of bulk volume occupied by fractures in the defined region.
- AREAMOD** Factor by which internally computed matrix-fracture interface areas is multiplied. The matrix-fracture area is computed by the relations given in Subsection A.6. Note that a value of zero for AREAMOD will decouple the matrix and fracture continua.
- XLM, YLM, ZLM** Average size of matrix blocks in x - y -, and z -directions respectively. If fracture spacing is very large corresponding to large matrix blocks in a given direction, the corresponding values of XLM, YLM, or ZLM may be set to zero, in which case the internally computed matrix-fracture surface area will be ignored in that direction.

Comment(s):

Read one region per line and terminate the read-sequence by reading a slash (/), asterisk (*), or period (.) in column 1. Overlapping specification of regions will not cause any error, with last entry taking precedence.

Examples:

```
DCMParameters
1 3 1 1 1 5 0.01 1. .1 .1 .1
/
```

2.2.2.6 Depths of Grid Blocks [DEPT_h]

Initialization Data

Keyword: DEPT_h

Optional

This keyword defines the depth of grid blocks. It can be used to set the depth of each block to define uneven topographies or a constantly dipping bed. If omitted, a depth of zero corresponding to a dip angle of zero is set for the top layer and other layer depths are computed by adding the thicknesses of the overlying layer or layers. This keyword should not be used with the unstructured grid option.

Read: DEPT_h IDEPTH DIP

DEPT_h Keyword for calculating the depth of a uniformly dipping formation.

IDEPTH Index for the method for specifying the depth.

- = 1 Use the dip of the formation to calculate depths
- = 2 Top layer depths are specified from which the other layer depths are computed by adding the thicknesses of the overlying layers
- = 3 Depths of all blocks are specified

DIP Dip in degrees along the x-axis. (Dip is formation inclination with respect to horizontal plane.) If IDEPTH > 1, the DIP is not used. The dip in the y-direction is assumed to be zero. For cylindrical system the dip must be zero.

Read the following additional data for IDEPTH > 1 in the following format.

If IDEPTH = 2

```
do J = 1,NY
  read() (H(I,J,1), I=1,NX)
end do
```

If IDEPTH = 3

```
do K = 1,NZ
  do J = 1,NY
    read() (H(I,J,K), I=1,NX)
  end do
end do
```

1. The previous read structure is as follows:
 - (a) Read NX values of depths for the top layer for row 1 ($J = 1, K = 1$).
 - (b) Repeat step (a) for successive rows ($J = 2, 3, \dots, NY$) for the top layer ($K = 1$) starting each row on a new line.
- If IDEPTH = 3, repeat steps (a) and (b) for successive planes ($K = 2, 3, \dots, NZ$) until all NZ planes are read in.
2. The depths are measured POSITIVE (INCREASE) DOWNWARD. The top layer corresponds to $K = 1$ and the bottom layer to $K = NZ$. That is, the layers are numbered from top to bottom. The depths are specified in units of meters.
 3. The read-in depth should be at the center of the upper surface of a block. The block center depths (halfway through the thickness) are computed internally by adding half the thickness to the read-in values.
 4. The calculated depths of lower layers ($K = 2, 3, \dots, NZ$) using option IDEPTH = 2 can introduce excessive errors if the formation is steeply dipping or highly undulating, in which case the option IDEPTH = 3 is recommended.
 5. All depths are to be specified with reference to the depth of block (1,1,1) to which HREF (read in with the Keyword GRID) is added internally.
 6. For a cylindrical system, all depths for a given layer must be constant. That is, the cylinder-axis must be vertical with zero formation dip.

Examples:

Constant Dip Specified (IDEPTH = 1).

DEPTH 1 10. ! designates 10 degree dip of the formation for option IDEPTH = 1.

Top Layer Depths Specified (IDEPTH = 2)

```
DEPTH 2
15 20 30 40 50 70 90 100 110 120
130 140 150 4*160 !(row = 1, Layer = 1)
20 25 35 45 55 75 95 110 120 130
140 160 180 4*200 !(row = 2, layer = 1)
. . . . .
. . . . .
100 120 130 140 150 160 170 180 190 200
220 230 240 4*250 !(row = NY, layer = 1)
```

If depths of all layers specified (IDEPTH = 3), the same data structure as the above is used for each successive layer.

2.2.2.7 Grid-Block Sizes [DXYZ]

Initialization Data

Keyword: **DXYZ**

Conditional

This keyword designates the size of grid blocks in $x(r)$ -, $y(\theta)$ -, and z -directions. It also specifies the choice of grid as to block-centered (default) or point-distributed (not implemented). This data set may be omitted if the grid block coordinates are specified with the keyword CXYZ or if UNSTRUCTURED grid geometry is used. For an unstructured grid, data associated with this dataset are ignored.

Read: DXYZ IGRID RW RE

Read: (DX(I), I = 1, NX)

Read: (DY(J), J = 1, NY)

Read: (DZ(K), K = 1, NZ)

DXYZ Keyword for reading grid-block sizes.

IGRID Index for grid-type.

= 0 block centered

= 1 Point-Distributed (not implemented)

= 2 Boundary node at the surface corresponding to CTOUGH (Nitao, 1989)

RW Inner boundary radius for cylindrical system [m].

RE Outer boundary radius for cylindrical system [m].
For Cartesian geometry, RW and RE are not required, and ignored if specified.

DX Block sizes in x -direction [m]. For a cylindrical system, DX designates the radius to block center from the axis of the cylinder.

DY Block sizes in y -direction [m]. For a cylindrical system, DY designates the sector angle of a block in degrees.

DZ Block thicknesses [m]. Note that the z -direction is positive downward with the top block numbered as 1 and the bottom block as NZ.

Comment(s):

For cylindrical geometry, fewer than NX nonzero values for DX may be read, in which case the rest will be computed internally based on logarithmic spacing. The inner radius RW must satisfy the inequality $RW < DX(1)$.

Values are read in order of DX, DY, and DZ starting DX, DY, and DZ each on a new line. Read NX nonzero values for DX, NY values for DY, and NZ values for DZ. In any case, whether DX(), DY(), and DZ() are zero or not, exactly NX, NY, and NZ values, respectively, must be read for DX(), DY(), and DZ().

For an unstructured grid, NX, NY, and NZ as read by the GRID keyword are not used for internal computations. However, values for DX, DY, and DZ are still read in corresponding to the values specified for NX, NY, and NZ in the GRID keyword. If either NX, NY, or NZ is zero, no value for DX, DY, or DZ may be read.

Examples:

Cartesian Geometry:

```

      igrid  rw  re
DXYZ  0      0  0
: dx(1) dx(2)....
1. 1. 1.5 1.5 2. 2. 3. 3. 5. 10.! x-direction
15. 15. 40.
: dy(1)
1.                                ! y-direction
: dz(1) dz(2) ...
10. 20. 30. 45. 60. 50. 50. 150.! z-direction

```

This example, designates block sizes for a Cartesian grid system of 13 blocks in the x-direction, 1 block in the y-direction, and 8 blocks in the z-direction.

Cylindrical Geometry:

```

: igrid      rw  re
DXYZ  0      .001 100. ! radial geometry with inner and outer radius of
:                                cylinder .001 and 100 m.
:
:      r(1) r(2)
:      .5  1.  11*0. ! only 2 values are specified. The rest will be
:                                computed internally.
:
: dy(1)
90.                                ! one angular sector of 90 degrees.
: dz(1)      dz(2) ...
10. 20. 30. 10. 20. 40. 100. 150.! z-direction

```

2.2.2.8 Equilibration [EQUilibration]

Initialization Data

Keyword: **EQUilibration**

Optional

This keyword sets the system initially in approximate capillary-gravity equilibrium for zero flux boundary conditions. The fluid velocity in all directions is assumed to be zero. That is, the gas and the liquid phase potentials are constant throughout the system. Use of this keyword overrides the pressure, temperature, and saturation specified by the keyword INIT.

Read: EQUIL DEPTH PDEPTH TDEPTH TGRAD PARAM IEQUIL

EQUIL Keyword for initial equilibration of the system.

DEPTH Reference depth at which gas phase pressure (PDEPTH) and temperature (TDEPTH) are specified [m].

In a two-phase system, if a water table (gas-water contact) exists within the system, it is recommended that DEPTH correspond to the depth of the water table. A water-table depth is defined as the highest depth at which 100 percent water saturation exists.

PDEPTH Specified gas phase pressure at the specified depth DEPTH [Pa].

TDEPTH Specified temperature at the specified depth DEPTH [°C].

TGRAD Temperature gradient (a constant) used to calculate temperature of each grid block [°C/m].

PARAM Parameter whose value is dependent on the variable IEQUIL. See its definition of IEQUIL in the next paragraph.

- = Gas saturation at depth = DEPTH, if IEQUIL > 0 [fraction]
- = Capillary pressure ($P_g - P_w$) at depth = DEPTH, if IEQUIL < 0 [Pa]
- = Pressure gradient for gas pressure in a two-phase or pure gas system, and liquid pressure for a pure liquid system (a constant) if IEQUIL = 0 [Pa/m]

IEQUIL Index for defining PARAM

- < 0, PARAM = capillary pressure specified at DEPTH
- > 0, equal to the sequential number defining the van Genuchten relative-permeability function defined by the PCKR keyword. The integer must be in the range of 1 to NST, where NST is the number of PCKR

functions read. The integer is used to calculate the capillary pressure corresponding to the given gas saturation, PARAM.
= 0, if PARAM = pressure gradient.

Examples:

:	depth	pdep	tdep	tgrad	param	iequil	
EQUIL	0	1.e5	.25.	.025	0.4	2	! equil with Sg specified
EQUIL	0.	1.e5	.25.	.0251.	e4	-1	! equil with cap. press.
EQUIL	0.	1.e5	.25.	.0259	800.	0	! equil with p-gradient.

2.2.2.9 Grid Geometry [GRID]

Initialization Data

Keyword: **GRID**

Required

The GRID keyword defines the grid geometry (radial, Cartesian, or unstructured), dual continuum model or single continuum, number of nodes in each direction, and other optional parameters.

Read: GRID GEOMETRY NX NY NZ IVPLWR IPVCAL IOUTPT GRAVITY PREF TREF
HREF

GRID Keyword defining grid geometry and optional parameters.

GEOMETRY Coordinate system geometry.

- = RADIAL for cylindrical geometry
- = XYZ for Cartesian geometry
- = UNSTRUCTURED grid
- = DCMRAD for dual continuum model formulation with cylindrical geometry
- = DCMXYZ for dual continuum model formulation with Cartesian geometry
- = DCMUNSTRUCTURED grid for dual continuum model formulation

NX Number of grid blocks in x - or r -direction.

NY Number of grid blocks in y - or θ -direction. For a cylindrical system, NY must be 1.

NZ Number of grid blocks in z -direction.
The variables NX, NY, and NZ are ignored for UNSTRUCTURED grid geometry, except for keyword DXYZ which uses these variables.

IVPLWR Index for vapor pressure lowering [see Eq. (A-8)].

- = 0 Do not invoke vapor-pressure lowering
- = 1 Invoke vapor-pressure lowering due to capillary suction

IPVICAL Index for calculating water pressure-volume-temperature properties. This option is available for temperatures up to 369 °C.

- = 0 Construct lookup tables using correlations
- = 1 Use correlations for H₂O properties

IOUTPT Index for output of Initialization Data.

- = 0 Suppress all initialization output
- = 1 Suppress initial porosity, permeability distribution in addition to items corresponding to the value = 2
- = 2 Suppress initial condition, transmissibility, and related output
- = 3 Print full initialization output

GRAVITY Gravitational acceleration vector [m/s^2] (default = 9.8068 m/s^2 , if < 0 , internally set to zero). Gravity is ignored if a negative value is assigned to it.

PREF Reference pressure for pore compressibility [Pa] [default = initial pressure of block (1,1,1)]

TREF Reference temperature for pore compressibility [$^{\circ}\text{C}$] [default = initial temperature of block (1,1,1)]

HREF Reference depth of grid block (1,1,1). That is, HREF specifies the depth of the first block (top). Other block depths are computed internally with reference to this depth. Note that the depth increases (positive) downward.

By appropriate assignment of NX, NY, and NZ, one-, two-, and three-dimensional problems may be defined. A zero dimensional (single block) problem can be defined by setting all $\text{NX} = \text{NY} = \text{NZ} = 1$. Computational limit on the maximum number of blocks in any direction and the total number of blocks can be specified by the user (see section on dimensioning and compilation).

For $\text{IPVCL} = 0$ a pressure-volume-temperature table is constructed for H_2O for a rapid table look-up procedure in subsequent calculations of fluid properties. The table is constructed at 2°C intervals for the range of $5\text{--}369^{\circ}\text{C}$ for saturated water, compressed liquid, and superheated water vapor.

PREF and TREF are used to calculate porosity change with pressure and temperature. It is assumed that the values read in for porosity are assigned at this reference pressure and temperature. If default values are used, the corresponding fields may be left blank or read as zeros.

Example:

```

: geometry nx ny nz ivplwr ipvcal ioutput gravity pref tref href
  GRID XYZ 21 1 32 0 0 1 0. 0. 0. 0.

```

This example, designates a Cartesian grid with $21 \times 1 \times 32$ nodes with no vapor pressure lowering, table look-up for H_2O properties, and default values for reference p , T , and depth. The comment line preceding the data line identifies the variables.

2.2.2.10 Initial Condition [INIT]

Initialization Data

Keyword: **INIT**

Required

The INIT keyword reads initial pressure, saturation, temperature, and mole fraction of component 2 (air). For two-phase regions, temperature is used to calculate the partial pressure of air in the gas phase which is used as a primary variable.

Read: INIT FN**Ustructured Grid Read:** M1 M2 INC P T SG XA PM TM SGM XAM**Structured Grid Read:** I1 I2 J1 J2 K1 K2 P T SG XA PM TM SGM XAM**INIT** Keyword for reading initial conditions.

FN File name from which the initial condition data are read (optional). The file name must have an extension of `.int` in lower case letters, but the extension should not be included in FN specification. The file name FN (excluding the extension) should not exceed 6 characters. The run will stop if the file name is misspelled or the file `fn.int` does not exist. (Default = blank space, in which case the data are read from the input file). The initialization data can be obtained from the METRA output file as cut-and-paste data (see keyword RSTArt).

M1, M2 Beginning and ending node numbers.**INC** Increment of node numbers. Default value for INC = 1.**I1, I2** First and last index in $x(r)$ -direction.**J1, J2** First and last index in $y(\theta)$ -direction.

K1, K2 First and last index in z -direction.
These indices define a region for which all properties are constant.

P Gas phase pressure for the defined region [Pa].**T** Temperature for the defined region [$^{\circ}$ C].**SG** Gas phase saturation for the defined region [fraction].

XA	Mole fraction of air in the defined region [fraction].
PM	Matrix gas phase pressure in matrix for the defined region [Pa].
TM	Matrix temperature for the defined region [°C].
SGM	Matrix gas phase saturation for the defined region [fraction].
XAM	Matrix mole fraction of air in the defined region [fraction].

The matrix data PM, TM, SGM, and XAM are ignored for a single continuum system. They are used only for equivalent continuum model, dual continuum model, and multiple interacting continuum options.

XA and XAM are independent variables only for a single-phase state and, therefore, they are ignored for a two-phase system.

Read as many lines as required to define the initial condition for the entire system, and terminate the sequence by reading a line with a slash (/), asterisk (*), or period (.) in column 1.

If two or more regions overlap, the last region read overrides the earlier ones.

Initial conditions must be specified for the entire system (for all grid blocks), otherwise results may be unpredictable because default values are not used. For the equivalent continuum model, dual continuum model, and multiple interacting continuum options, P, T, SG, and XA correspond to values for the fracture continuum.

Data corresponding to this keyword will be ignored if the EQUIL keyword is specified.

Example:

```

: i1  i2  j1  j2  k1  k2  p    t    sg  xa  pm  tm  sgm  xam
  1   64  1   32  1   1  1.0e5 25.0 0.9 0.  1.e5 25.  .30  0.
.   .   .   .   .   .   .   .   .   .   .   .   .   .
.   .   .   .   .   .   .   .   .   .   .   .   .   .
.   .   .   .   .   .   .   .   .   .   .   .   .   .
/

```

2.2.2.11 Klinkenberg Gas Slippage Parameters [KLINKenberg]

Initialization Data

Keyword: **KLINKenberg**

Optional

This keyword assigns a table of Klinkenberg parameters b as a function of absolute rock permeability. Increased gas flow rate due to gas slippage is accounted for by this parameter.

Read: KLINKenberg

Read: PERMT BKLINT

...
...
...
*

KLIN Keyword for reading the Klinkenberg parameters.

PERMT Absolute rock permeability [m²].

BKLINT Klinkenberg constant for a given gas corresponding to permeability PERMT [Pa].

Read a table of BKLINT as a function of PERMT with increasing PERMT. This table is used for permeability in $x(r)$ -, $y(\theta)$ -, and z -directions to calculate BKLINT using a $\log(\text{PERMT})$ -linear(BKLINT) interpolation.

Sufficient values of PERMT should be read to cover the entire range of permeability values assigned by PHIK keyword. If the table does not extend to cover the full range, the end values of BKLINT are assigned to the permeability values which fall beyond the table range. If BKLINT is constant for the entire permeability range, or if the permeability is constant for the entire system, a single table entry should be sufficient, in which case PERMT is ignored. Read as many entries as desired and terminate the reading sequence by reading a line with slash (/), asterisk (*), or period (.) in column 1.

Note the gas slippage effect is most pronounced at low permeability ($< 1.e-15$) and low pressures. Thus, if the permeability values are greater than tens of millidarcy, this phenomenon may be ignored. On the other hand, permeability values below 1 millidarcy may cause an appreciable slippage effect of gas.

For the single-phase liquid case or for pure conduction problems, these data are not used.

Enhanced gas permeability due to gas slippage is related to absolute rock permeability by the relation:

$$K_{\text{gas}} = K_{\text{abs}} \left(1 + \frac{b}{\bar{p}} \right) \quad (2-1)$$

where

$$b = \text{BKLINT} [\text{Pa}] \quad (2-2)$$

$$\bar{p} = \text{mean gas phase pressure} [\text{Pa}] \quad (2-3)$$

$$K_{\text{abs}} = \text{absolute rock permeability} [\text{m}^2] \quad (2-4)$$

Example:

KLINKenberg	
:Permt	Bklint
:m2	Pa
1.e-18	8.e5
1.e-17	5.e5
1.e-16	2.e5
1.e-15	.7e5
1.e-14	.3e5
1.e-13	.13e5
1.e-12	.05e5
*	

2.2.2.12 Single-Phase Liquid System [LIQUid]

Initialization Data

Keyword: **LIQUid**Conditional

The LIQUid keyword designates the system to be all liquid and isothermal. In this case, the computational work and the memory requirement are reduced by more than an order of magnitude. In addition, this option enables simulation of a nonaqueous fluid.

Read: LIQUid DWS VISW CWS

LIQUid Keyword for designating the system to be isothermal and single-phase liquid.

DWS Density of liquid [kg/m^3] (default = water density computed internally).

VISW Liquid viscosity [kg/m/s] (default = water viscosity computed internally).

CWS Liquid compressibility [$1/\text{Pa}$] (default = water compressibility computed internally).

The default values correspond to the temperature and pressure of block (1,1,1).

Example:

```
Liquid 970 0 0
```

In this example, the density of liquid is assigned a value of 970 kg/m^3 , while the viscosity and the compressibility are taken as that of water from the internally calculated pressure-volume-temperature properties.

2.2.2.13 Multiple Interacting Continua [MINC]

Initialization Data

Keyword: **MINC**

Conditional

The **MINC** option is not implemented in this version.

2.2.2.14 Rock Saturation Characteristic Properties [PCKR]

Initialization Data

Keyword: **PCKR**

Required

This keyword specified the relative permeability and capillary pressure characteristics for different rock types. The characteristic curves included are equivalent continuum, van Genuchten, Linear, Tabular, and Corey Equations.

Read: PCKR FN**Read:** NO TYPE SWIRM RPMM ALPHAM SWEXT SGC IECM**If IECM > 0:****Read:** SWIRF RPMF ALPHAF PHIM PHIF PERMM PERMF**PCKR** Keyword defining relative permeability and capillary pressure characteristic curves.

FN File name from which data for potential properties are read (optional). The file name must have an extension of `.pck` in lowercase letters, but the extension should not be included in the FN specification. The file name FN (excluding the extension) should not exceed six characters. The run will stop if the file name is misspelled or the file `fn.pck` does not exist. (Default = blank space, in which case the data are read from the input file).

NO Sequential number.**TYPE** Three character string identifying the type curve.

- = VAN-gen, van Genuchten Curves
 - = LINear, Linear curve
 - = TABular, Data are read in tabular form
 - = COREy, Corey's curves
-

If TYPE = Van-Gen read the following:

SWIRM Irreducible liquid saturation [see Eq. (A-1)] $\{K_{r_l} = 0$ for saturations below the residual saturation [see Eq. (A-4)]} [fraction]. For the equivalent continuum model, it represents the irreducible liquid saturation for the matrix.

- RPMF** Exponent λ in van Genuchten equation for fracture.
- RPMM** Exponent λ in van Genuchten equation [see Eq. (A-3)]. For the equivalent continuum model, RPMM represents the exponent for the matrix.
- ALPHAM** Parameter α in van Genuchten equation [1/Pa] [see Eq. (A-1)]. For the equivalent continuum model, ALPHAM represents the matrix parameter.

The preceding three variables refer to the matrix continuum for equivalent continuum model formulation, IECM > 0.

- SWEXT** Saturation (capillary pressure) cutoff parameter.
- ≥ 0 Liquid saturation below which the capillary pressure is calculated based on the slope dP_{cw}/dS_w evaluated at SWEXT. SWEXT must be greater than SWIRM. Default value for SWEXT = SWIRM+0.05. A value of SWEXT close to SWIRM may result in performance degradation. The effect is likely to be more severe with vapor pressure lowering option. SWEXT is set internally for IECM = 1 based on a cutoff value for the capillary pressure of 8.895e7 Pa. This approach is similar to that used in VTOUGH (Nitao, 1989).
- < 0 Cutoff value for capillary pressure [Pa]. This parameter is ignored if IECM = 1.

Performance depends sensitively on how the capillary pressure cutoff is set. Recommended values are -1.0e8 for RPMM<0.3, 0 otherwise.

- SGC** Critical (immobile) gas saturation [fraction].
- IECM** Index for invoking the equivalent continuum model. Available only for van Genuchten functions. Equivalent continuum model option should not be used with dual continuum model or multiple interacting continuum options.
- = 0 Do not invoke the equivalent continuum model
- = 1 Invoke the equivalent continuum model using unequally spaced saturation versus P_c/K_r tables that are generated internally similar to VTOUGH (Nitao, 1989)
- = 2 Equivalent continuum model with equally spaced saturation tables generated internally
- = 3 User-specified PCKR tables for equivalent continuum model

- SWIRF** Irreducible liquid saturation for the fracture [fraction].
- ALPHAF** Van Genuchten parameter α for the fracture [1/Pa] [see Eq. (A-1)].
- PHIM** Matrix porosity [fraction].

PHIF Fracture porosity [fraction].

PERMM Matrix permeability [m^2].

PERMF Fracture permeability [m^2].

If IECM = 3:

Read: (SWT(l), FKRWT(l), FKRGT(l), PCWT(i), $i = 1, nn$)

SWT Liquid saturation ($0 \leq \text{SWT} \leq 1$) [fraction].

FKRWT Liquid relative permeability corresponding to SWT.

FKRGT Gas relative permeability corresponding to SWT.

PCWT Liquid-gas capillary pressure [Pa].
This is a general case in that any functional forms of the relative permeability and the capillary pressure may be used to generate a table and be entered with this option.

Read one entry per line with a total of nn entries followed by a line with one of the terminators a slash (/), asterisk (*), or period (.) in column 1.

SWT must cover the range from SWIRM to 1 and must be read in ascending order.

A sufficient number of entries should be read to define a smooth variation in the relative permeability and the capillary pressure values.

If TYPE = LINEar, read the following [see Eq. (A-7)]:

SWIRM Irreducible liquid saturation ($K_{rw} = 0$ below irreducible saturation).

RPMM Not used (simply read zero, not blank).

ALPHAM Not used (simply read zero, not blank).

SWEXT Capillary pressure at zero liquid saturation [Pa].

SGC Critical (immobile) gas saturation [fraction].

IECM 0

The relative permeabilities are linear functions ranging from 0 to 1 such that $K_{rw} = 0$ at or below SWIRM liquid saturation and $K_{rg} = 0$ at or above $(1 - \text{SGC})$

liquid saturation. The capillary pressure is linear between 0 to SWEXT corresponding to liquid saturations of 1 and 0. Not applicable to the equivalent continuum model.

If TYPE = TABular, read the following:

- SWIRM** Irreducible liquid saturation ($K_{rw} = 0$ below it) [fraction].
- RPMM** Not used (simply read zero, not blank).
- ALPHAM** Not used (simply read zero, not blank).
- SWEXT** Same as for TYPE = 1.
- SGC** Critical (immobile) gas saturation [fraction].
- IECM** 0.
- Read:** (swt(i), fkrwt(i), Fkrgt(i), Pcwt(i), i = 1,nn)
- SWT** Liquid saturation ($0 \leq \text{SWT} \leq 1$) [fraction].
- FKRWT** Liquid relative permeability corresponding to SWT [m^2].
- FKRGT** Gas relative permeability corresponding to SWT [m^2].
- PCWT** Liquid-gas capillary pressure [Pa].

This is a general case in that any functional forms of the relative permeability and the capillary pressure may be used to generate a table and entered with this option.

Read one entry per line with a total of nn entries followed by a line with one of the terminators a slash (/), asterisk (*), or period (.) in column 1.

SWT must cover the range from SWIRM to 1 and must be read in ascending order.

A sufficient number of entries should be read to define a smooth variation in the relative permeability and the capillary pressure values.

If TYPE = COREy, read the following [see Eq. (A-6)]:

- SWIRM** Irreducible liquid saturation ($K_{rw} = 0$ below the irreducible saturation).
- RPMM** Not used (simply read zero, not blank).

ALPHAM Not used (simply read zero, not blank).

SWEXT Not used (simply read zero, not blank).

SGC Critical (immobile) gas saturation [fraction].

IECM 0.

The relative permeability is computed using the following function.

```
sstar=(usw-swirm)/(1-swirm-sgc)
fkrw=sstar**4
fkrge=(1-sstar*sstar)*(1-sstar)**2
```

The capillary pressure is internally set to zero for this case. As such, this option is not applicable to the equivalent continuum model.

Same type-curves with different parameters may be read in as often as desired. The sequential number does not have to start in ascending order but should cover the range of the number of lines read. That is, if there are 10 curves designated, the number should range between 1 to 10 in any desired order with each set of parameters on a new line.

Read many entries as desired and terminate the reading sequence by reading a line with slash (/), asterisk (*), or period (.) in column 1.

Note that the data on the second line should be read only if IECM > 0.

Example:

```
PCKR
:   No.  type  swir  lambda  alpha  swext  sgc  iecm
:   1   Van   .01   .75   1.31e-5  0.    0.    1
:   swirf  lambdaf alphaf  phim   phif   fkm   fkf
.2  .36   8.    4e-7  .3    1.e-3  1.e-18 1.e-12
:   Van   .01   .75   1.31e-5  0.    0.    1
.3  .44  6.1e-7 .35  1.e-3  1.e-16 1.e-12
/ ! data terminator
```

2.2.2.15 Rock Properties [PHIK]

Initialization Data

Keyword: **PHIK**

Required

This keyword assigns block volume, rock porosity, permeability, the associated relative permeability-capillary pressure characteristics, and thermal properties.

READ: PHIK FN

Unstructured Grid Read: M1 M2 INC IST ITHRM VB POR PERMX PERMY PERMZ
PORM PERMM ISTM ITHRMM

Structured Grid Read: I1 I2 J1 J2 K1 K2 IST ITHRM VB POR PERMX PERMY
PERMZ PORM PERMM ISTM ITHRMM

PHIK Keyword for reading porosity/permeability data.

FN File name from which porosity/permeability data are read (optional). The file name must have an extension of .phk in lowercase letters, but the extension should not be included in FN specification. The file name FN (excluding the extension) should not exceed six characters. The run will stop if the file name is misspelled or the file `fn.phk` does not exist. (Default = blank space, in which case the data are read from the input file).

M1, M2 Beginning and ending node numbers.

INC Increment of node numbers (default = 1).

I1, I2 First and the last index of a region in $x(r)$ -direction.

J1, J2 First and the last index of a region in $y(\theta)$ -direction.

K1, K2 First and the last index of a region in z -direction.
The properties of a region bounded by the indices I1, I2, J1, J2, K1, K2 are defined to be constant.

IST Characteristic curve number for relative permeability and capillary pressure. The curve numbers are identified by the sequential numbers read in PCKR data.

ITHRM Thermal properties data set number read in by the keyword THERmal. The sequential number of rock thermal properties must be assigned.

VB	Block volume [m ³]. If read as zero, it is computed internally based on the grid block sizes (DX, DY, DZ). For unstructured geometry, VB must be specified through this keyword.
POR	Porosity [fraction].
PERMX	x(<i>r</i>)-directional absolute rock permeability [m ²].
PERMY	y(<i>θ</i>)-directional absolute rock permeability [m ²].
PERMZ	z-directional absolute rock permeability [m ²].
PORM	Matrix porosity [defaults to PHIM(IST)].
PERMM	Matrix permeability [m ²] [defaults to FKM(IST)].
ISTM	Matrix characteristic curve number for relative permeability and capillary pressure. The curve numbers are identified by the sequential numbers read in PCKR data.
ITHRMM	Matrix thermal properties data set number read in by the keyword THERmal. The sequential number of rock thermal properties must be assigned.

In case the equivalent continuum model formulation is invoked, if any of the porosity or permeability values are read as zero, they are set to the values assigned by the PCKR keyword. For a nonequivalent continuum model system, the values are used as specified here. For the equivalent continuum model formulation, PERMX, PERMY, and PERMZ refer to the values for fracture continuum where PERMY and PERMZ are internally set equal to PERMX, as the current implementation of the equivalent continuum model option applies only to isotropic systems. The quantities POR and PORM for dual continuum model are intrinsic porosities of the fracture and matrix. For the equivalent continuum model, they refer to bulk porosities.

In dual continuum model mode, fracture permeabilities are intrinsic not bulk properties. Intrinsic permeability is bulk permeability divided by SIGMAF (see page 2-14).

ISTM and ITHRMM are used only for dual continuum model formulations.

Read as many entries as desired and terminate the reading sequence by reading a line with a slash (/), asterisk (*), or period (.) in column 1. Termination with a negative integer or with value -1 or -2 activates other options that are discussed in the following paragraphs. These options apply only to single-continuum permeability systems.

If regions overlap, the last region read overrides the former ones.

If the data are not specified for the entire system (for all grid blocks), it may cause unpredictable results.

Termination with I1 = -1

This option permits a more convenient way to assign the values for porosity, permeability, gas saturation, and the relative permeability functions for generally heterogeneous rock properties. This option does not permit reading matrix data. One or more of these properties must be created and saved on a separate file that must be named as filename FN. The data in file FN should be in the following format:

```
KEYWORD  FAC  FKY  FKZ
```

```
data in free format corresponding to this keyword
```

```
. . . . .
. . . . .
. . . . .
```

```
Return
```

The input variables KEYWORD, FAC, FKY, and FKZ have the following meanings:

KEYWORD Keyword for defining data.

PERMeability	Read x-direction permeability.
PORosity	Read porosity, fraction.
SGINit	Read the initial gas saturation.
SATF	Read relative permeability/capillary function table number. They must be read as integers.

FAC Factor by which the read-in values are to be multiplied. This is especially helpful in converting data to proper units. This factor is ignored for keyword SATF.

FKY, FKZ Factors by which x-direction permeability are to be multiplied to obtain y- and z-direction permeabilities. These are ignored for other keywords.

The values corresponding to the keywords may be read in any order. The last line on the file must have a Return statement. These values override any data specified in the INIT keyword.

The data are read in the order of increasing i, j, and k indices. For example, the porosity array is read as

```
do k = 1,nz
  do j = 1,ny
    read (lfn,*) (por(i,j,k), i = 1,nx)
  end do
end do
```

It should be ensured that values for each elements are assigned. Permeability in y- and z-directions are automatically computed as a factor of x-direction values. If fky or fkz are read as zero, the corresponding directional permeability is computed as zero. Comments are not permitted within the grid.inp file.

Example:

```

Permeability 1. .5 .1
1.e-12 1.e-11 2.e-13 4.e-13 .....(i= 1, nx, j = 1, k = 1) 2.e-13 3.e-12
1.e-11 1.e-15 .....(i= 1, nx, j = 2, k = 1) . . . . .
3.1e-11 4.6e-12 2.9e-12 3.e12 ... (i= 1, nx, j = ny, k = 1) 1.1e-12 2.3e-14
3.1e-15 3.e-12...(i= 1, nx, j = 1, k = 2) 2.e-11 3.e-11 5.e-11 6.e-13
...(i= 1, nx, j = 2, k = 2) . . . . .
7.e-11 8.e-12 9.e-13 5.e-11 ... (i= 1, nx, j = ny, k = 2) . . . . .
. . . . .
. . . . .
5.e-13 5.e-12 5.e-12 3.e-14 .....(i= 1, nx, j = ny, k =nz)
Porosity 1. porosity values in the same pattern as the above

Sginit 1. gas saturation values in the same pattern as the above

RETURN
    
```

The lines in parentheses should not be included in the `fn.phk` file. They are shown here for explanatory purposes only.

Termination with I1 = -2

In this case, the permeability values are internally generated using a random number generating algorithm. The indices I2 and J1 have the following additional meaning next.

- I2:** n size of equal permeability cluster
- J1:** $dn dx$ for specifying permeability and porosity fields.
- = 0** Compute permeability field only
- = 1** Compute correlated porosity and permeability

The permeability is computed from the relation

$$k_n = N_B \bar{k} \frac{R_n}{\sum_{n'} R_{n'}} \tag{2-5}$$

with random number R_n . The average permeability \bar{k} of the medium is taken from PERMX. The permeability correlated porosity is computed from the relation

$$\phi_n = \frac{k_n \bar{\phi}}{k} \tag{2-6}$$

The average porosity of the medium is taken from PROM.

Example:

PhiK

:	i1	i2	j1	j2	k1	k2	iist	ithrm	vb	porm	permx	permy	permz
	1	100	1	100	1	1	1	1	0.	0.5	1.e-12	1.e-12	1.e-12
	-2	2	0	100	1	1	1	1	0.	0.5	1.e-12	1.e-12	1.e-12
:	0												

2.2.2.16 Rock Thermal Properties And Binary Diffusion Data [THERmal]

Initialization Data

Keyword: **THERmal**

Required

The keyword THERmal assigns the thermal properties of the rock and binary diffusion parameters.

- Read:** THERmal
- Read:** NO RHO CPR CKDRY CKSAT CRP CRT TAU CDIFF CEXP ENBD
- THER** Keyword for reading the thermal properties.
- NO** Sequential number of the data set.
- RHO** Rock density [kg/m³].
- CPR** Rock specific heat [J/kg-K].
- CKDRY** Thermal conductivity of dry rock [see Eq. (A-9)] [J/s/m-K] (default = CKSAT).
- CKSAT** Thermal conductivity of liquid saturated rock [see Eq. (A-9)] [J/s/m-K] (default = CKDRY).
- CRP** Pore compressibility, $(\partial\phi/\partial p)/\phi$, with pressure at constant T [1/Pa] (default = 0).
- CRT** Absolute value of pore expansivity, $(\partial\phi/\partial T)/\phi$, with temperature at constant pressure [1/T] (default = 0).
- TAU** Tortuosity for binary diffusion (default = 0).
- CDIFF** Vapor-air diffusion coefficient [m²/s] [see Eq. (A-16)] (default = 2.13e-5 m²/s).
- CEXP** Exponent for binary diffusion [see Eq. (A-16)] (default = 1.8).
- ENBD** Enhanced binary diffusion coefficient [see Eq. (A-16)] (default = 0).
- = 0** enhanced binary diffusion not invoked
- > 0** invoke enhanced binary diffusion

The sequential number does not have to start in ascending order but should cover the range of the number of lines read. That is, if there are 10 rock-types designated, the number should range from 1 to 10 in any desired order with each set of parameters on a new line.

Read as many entries as desired and terminate the reading sequence by reading a line with a slash (/), asterisk (*), or period (.) in column 1.

Example:

```
Thermal
: rho  cpr  ckdry  cksat  crp  crt  tau  cdiff  cexp  enbd
1 2580. 840. 1.7  2.1 0.  0.  .5  2.13e-5 1.8  0
```

2.2.3 Recurrent Data Keywords

Recurrent data can be changed with time and include such items as the method of solution, source/sink tables, time step sizes, output frequency, boundary condition specifications, etc. A given type of data will remain effective until it is modified or replaced by a new set at subsequent time intervals. Thus, the method of solution may be kept fixed once defined initially, but output may be changed as desired during different time intervals. All data between the RECUrrent data and the first TIME keyword or between two consecutive TIME keywords constitutes one set of RECUrrent data. The keywords associated with RECUrrent data are as follows:

AUTO step	RSTART
BCONdition	SOLVe
DEBUg	SOURce
ENDS	STEADy
LIMIt	TIME
OUTPut	TOLR
PLOTs	
RECUrrent	

The keywords may be read in any order, EXCEPT the RECUrrent keyword that must be read first. When a TIME keyword is encountered, it is assumed that all the recurrent data have been assigned or changed as desired previous to the occurrence of the TIME keyword. The calculation proceeds until the target time assigned on the TIME keyword is reached. The last keyword in the data set must be the ENDS keyword that signals the completion of a run. The keywords are presented in alphabetical order for convenience.

2.2.3.1 Automatic Time Step Control Data [AUTOstep]

 Recurrent Data
Keyword: **AUTO step**

Optional

This keyword will override the default parameters used for automatic time step size calculations. It is best to leave the default parameters unchanged unless they are unsatisfactory based on the performance of a run or user experience with a specific problem.

Read:	AUTOstep DPMXE DSMXE DTMPMXE DP2MXE TACCEL IAUTODT FAC1
AUTO	Keyword for amending automatic time step size calculation parameters
DPMXE	Estimated maximum pressure change in any grid block during a time step [Pa] (default = .10e5 Pa)
DSMXE	Estimated maximum saturation change in any grid block during a time step (default = .04).
DTMPMXE	Estimated maximum temperature change in any grid block during a time step [°C] (default = 5°C).
DP2MXE	Estimated maximum air-phase pressure change in any grid block during a time step [Pa] (default = .10e4 Pa).
TACCEL	Acceleration parameter for automatic time step size calculation for IAUTODT = 1; for IAUTODT = 0, TACCEL is not used (default value for TACCEL = 1.e-4)
IAUTODT	Switch for time-stepping algorithm <ul style="list-style-type: none"> = 0 Algorithm based on estimated maximum changes in field variables given above is used for automatic time step calculations (recommended) = 1 Algorithm based on time derivative of field variables is used. Requires TACCEL
FAC1	Factor which the ratios DSMXE/DSMX, DPMXE/DPMX, etc., should not exceed. (default = 0.5) See LIMIt keyword. (Recommended value 0.5<FAC1<0.7). If any of these ratios exceed FAC1, then DSMXE, DPMXE, etc. are reset internally to satisfy this condition.

Note that the estimated values for changes in primary variables are used to calculate the next time step size and do not guarantee that the actual changes will not exceed these limits. An

absolute upper limit on changes is specified by the LIMIt keyword. These values will remain in effect until they are modified by any of the subsequent recurrent data set entries.

Example:

```
:      dpmxe  dsmxe  dtmpmxe  dpamxe  taccel  iauto  fac1
Auto Step  1.e4  .03 3.  1.e4
```

2.2.3.2 Boundary Condition Data [BCON]

Recurrent Data

Keyword: **BCON**

Conditional

This keyword assigns boundary conditions that can be changed at subsequent time intervals. The boundary conditions include both Dirichlet and Neumann types. For Neumann conditions, only liquid flux may be specified. For steam, or two-phase mixture of steam and liquid water, use source keyword to assign the desired flux. Boundary conditions may not be specified on faces separated by a single grid block. For example, for a two-dimensional x-z cross section, the boundary condition on the FRONT and BACK are not permissible. Zero flux boundary conditions are assumed as default on all faces.

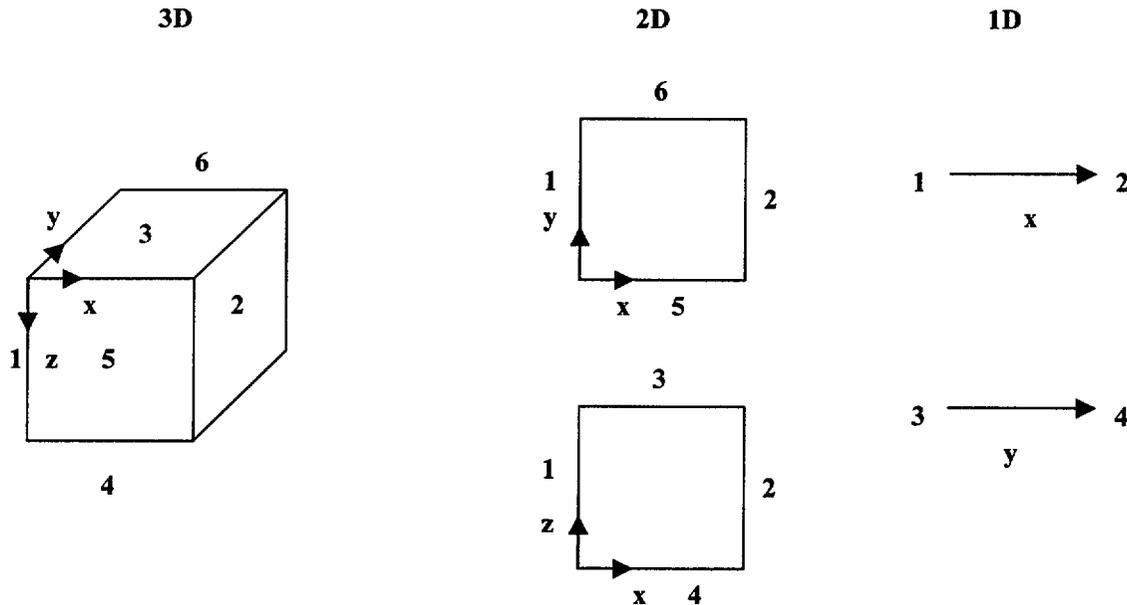


Figure 2-2. Boundaries of Computational Domain in Cartesian Coordinates

Read: BCON NBC FN

Unstructured Grid Read: ITYPE IPERMBC M1 M2 INC DISTBC AREABC DELHBC

Structured Grid Read: ITYPE IFACE I1 I2 J1 J2

Read: TIMBC QBC PBC TBC SGBC XABC EMSIVT

Dual Continuum Model Formulation Read: TIMBC QBCF PBCF TBCF SGBCF XBCF
EMSIVTF

- BCON** Keyword for assigning boundary conditions.
- NBC** Number of boundary conditions.
- FN** File name from which the time varying boundary condition data are read (optional). The file name must have an extension of `.bc` in lower case letters, but the extension should not be included in FN specification. The file name FN (excluding the extension) should not exceed six characters. The run will stop if the file name is misspelled or the file `fn.bc` does not exist. (Default = blank space, in which case the data are read from the input file).
- ITYPE** Type of boundary condition.
- = 1 Dirichlet (constant field variables)
 - = 2 Neumann (constant liquid flux)
 - = 3 Liquid velocity flux
 - = 4 Radiation heat flux only
 - = 5 Mixed (specified gas pressure, temperature and liquid flux)
 - = 6 Free drainage
- IPERMBC** Permeability direction at the boundary. Values must be 1, 2 or 3 corresponding to the permeability in x-, y-, and z-directions.
- M1, M2** Beginning and ending node numbers.
- INC** Increment of node numbers over which the boundary condition is imposed.
- DISTBC** Distance from the boundary to the block center [m].
- AREABC** Area of block surface over which the boundary condition is imposed [m²].
- DELHBC** Elevation difference between the boundary condition surface and the connecting node center. DELHBC is positive if the depth of the node is greater than the boundary surface, otherwise it is negative. It is defined as
- DELHBC = node depth - boundary surface depth.
- Default values for DISTBC and AREABC will be internally set to DIST1 and AREA in the specified permeability direction. The latter parameters were assigned by keyword CONNECTIONS in initialization data.
- IFACE** Surface at which the boundary condition is imposed (see Figure 2-2).

- = RIGHT, right face, that is at $I = NX$ (only applies if $NX > 1$)
- = LEFT, left face, that is at $I = 1$ ($x = r = 0$) (only applies if $NX > 1$)
- = TOP, top surface, that is at $K = 1$ (only applies if $NX > 2$)
- = BOTTOM, bottom surface, that is at $K = NZ$ (only applies if $NX > 2$)
- = FRONT, front surface of the block at $J = 1$ (only applies if $NY > 1$)
- = BACK, back surface of the block at $J = NY$ (only applies if $NY > 1$)

I1, I2, J1, J2 Indices defining the region on the designated face where the conditions are to be imposed.

TIMBC Time [seconds].

QBC = not used if $ITYPE = 1$ or $ITYPE = 6$
 = liquid flux rate [$\text{kg}/\text{m}^2/\text{s}$], if $ITYPE = 2$ or $ITYPE = 5$
 = liquid velocity [m/year], if $ITYPE = 3$; Flux and velocity are positive if mass is entering the system and negative if mass is leaving the system

PBC Gas phase pressure at the designated surface [Pa]. If $PBC \leq 0$, then the boundary represents a zero mass flux boundary and heat flux dry conduction only. In this case, SGBC and XABC are not used. If $SGBC = 0$, $PBC =$ water phase pressure.

TBC Temperature at the designated surface [$^{\circ}\text{C}$] ($ITYPE = 1,5,6$) and temperature of incoming liquid ($ITYPE = 2,3$).

SGBC Gas phase saturation at the designated surface.

XABC Mole fraction of air at the surface. This is required only for single phase systems when $SGBC = 0$ or 1 .

EMSIVT Emissivity for radiation heat transfer $0 \leq EMSIVT \leq 1$.

PBCF, TBCF, SGBCF, XABCF, and EMSIVT for the dual continuum model formulation, are fracture parameters corresponding to PBC, TBC, SGBC, XABC, and EMSIVT. The latter variables are assigned to the matrix continuum for a dual continuum model system.

The variables PBC and SGBC (also PBCF and SGBCF) are not used for Neumann boundary condition, that is for $ITYPE = 2$. Also, SGBC and XABC are not used for pure liquid isothermal systems defined by LIQUID keyword. For the equivalent continuum model they correspond to the average values of matrix and fracture. For $ITYPE = 4$, all variables except temperature and emissivity are ignored. If $ITYPE = 1$ and $EMSIVT > 0$, heat transfer by conduction, convection, and radiation is taken into account. $ITYPE = 4$ considers only radiation heat transfer, $q_{\text{rad}} = \sigma EMSIVT (T_1^4 - T_2^4)$.

The ITYPE = 6 boundary condition represents free drainage from a seepage face. It is only applicable for boundaries with DELHBC < 0. TBC and PBC are specified.

In dual continuum model mode the liquid flux rate in fractures is per intrinsic area not bulk area.

Read one line defining each region followed by a set of time varying input data terminated with a slash (/), asterisk (*), or period (.) in column 1. The number of entries and the time interval in each table (if more than one table) need not be the same.

Example:

```
Bcon 2
: itype  iface  i1  i2  j1  j2
   1      Right  1  10  1  5
: timebc  qbc   pbc   tbc  sgbc  xabc
   0.     0.   1.1e5  30   .4    0
/
: itype  iface  i1  i2  j1  j2
   3      Left  1  10  1  5
: timebc  qbc   pbc   tbc  sgbc  xabc
   0.     1.e-4 1.0e5  30   0.    0.
/
```

2.2.3.3 Maximum Time Step Limit [LIMIT]

 Recurrent Data
Keyword: **LIMIT**

Optional

This keyword modifies the default values that are used in limiting the maximum change in the primary variables during a time step. If during any time step the maximum change in a primary variable exceeds the value defined by **LIMIT** data (or the default values), the time step is successively cut (up to a maximum of 25 times) to ensure it is within these specified limits. If a cut in the time step results in a new time step that is > 0.9 of the original time step, the time step will not be cut, in which case the solution vector will slightly exceed **LIMIT** data. This is done to avoid resolving the step with only a small difference in the time step size.

Read: **LIMIT** **DPMX** **DSMX** **DTMPMX** **DPAMX** **DTMN** **DTMX** **DTFAC**

LIMIT Keyword for modifying the default values (or earlier specified) for maximum change of solution vector.

DPMX Maximum change in pressure over a time step in any block [Pa] (default = $5.e4$ Pa).

DSMX Maximum change in saturation over a time step (default = 0.10).

DTMPMX Maximum change in temperature over a time step [T] (default = 10°C).

DPAMX Maximum change in partial air pressure over a step [Pa] (default = $.5e4$ Pa).

DTMN Minimum time step size allowed with units as specified on **TIME** or **STEADy** keyword (default = 1 sec).

DTMX Maximum time step size allowed with units as specified on **TIME** or **STEADy** keyword (Default = $3.15e9$ sec.) **DTMN** and **DTMX** are in the same units as the units for the time-step size (see **TIME** keyword).

DTFAC Factor by which a time step will be reduced if the solution failed to converge in a specified number of Newtonian iterations. A time step will be successively cut up to 25 times, after which the run will be terminated with an error message. **DTMN** and **DTMX** control the automatic time step size calculations, however, there is no lower limit of time step size during the time step cuts (default value for **DTFAC** = 0.334).

Note that **DPMXE**, **DSMXE**, **DPAMXE**, and **DTMPMXE** must not exceed **FAC1** times **DPMX**, **DSMX**, **DPAMX**, and **DTMPMX**. The former are specified by **AUTO** step keyword (see **AUTO** step).

Example:

: Limit	dpmx	dsm	dtmpmx	dp2mx	dtmn	dtmx	dtfac
	5.e4	0.05	5.0	1.e5	1.6-6	1.e4	0.5

2.2.3.4 Output [OUTPut]

Recurrent Data

Keyword: **OUTPut**

Optional

This keyword enables output of desired variables at specified time intervals or at specified target times. The frequency of output may be changed with repeated use of this keyword in subsequent Recurrent Data sets.

Read: OUTPut A=l B=m C=k G=m L=n P=n Q=j S=k T=i V=k Y=n

OUTPut Keyword for specifying output frequency.

A=1 All the important arrays in tabular form.

B=m Boundary condition fluxes summary.

C=k Output of convergence summary.

G=m Output of gas saturation array.

L=n Output of liquid saturation array.

P=n Output of pressure array.

Q=j Source/sink summary.

S=k Frequency of one-line summary output on the screen.

T=i Output of temperature array.

V=k Output of all directional velocity arrays.

Y=n Output of mole fraction of air in the gas phase.

Integers n, m, etc., following the equal sign designate the frequency of output. If the integer (say m) is negative, the output will be produced at every abs(m)th time step. If m is positive, it will be produced at every mth target time (see TIME keyword for the definition of target time). If output option A=l (where l is an integer as defined above) is specified such that l is a multiple of n, m, etc., for any of the other variables the output corresponding to these variables will not be produced, as A prints out all the variables in tabular form. The user should become familiar with these options to properly manipulate the output as desired.

Examples:

- OUTPUT A=1 Print all variables at every target time.
- OUTPUT C=-1 A=2 Print the convergence summary at every time step and
rest of the variables at every second target time.
- OUTPUT V=1 C=1 T=2 G=2 Output velocities and the convergence summary at every
target time, the temperature and gas saturations at
every second target time.

2.2.3.5 Plotting Results [PLOTS]

Recurrent Data

Keyword: **PLOTS**

Optional

This keyword designates the frequency of writing plot/graphic files for spatial and time-history post processing. This keyword is currently valid for structured grid only.

Read: PLOTS IPLOTS IPRNVEL MXNDPLT

Read: (NDPLTS (I), I=1, MXNDPLT)

PLOTS Keyword for reading plots/graphic files output.

IPLOTS Flag for setting plot frequency.

0 No graphic/plot files requested

n<0 Frequency in number of time steps for writing graphic files

m>0 Frequency in number of target times for writing graphic files. Integers m and n have absolute values <99999

IPRNVEL Flag for printing fluid velocities.

= 0 Fluid velocities not printed

= 1 Print fluid velocities at node centers

= 2 Print fluid velocities at block interfaces

= 3 Print fluid velocities at both node centers and block interfaces

MXNDPLT Number of nodes at which time-history data is stored.

NDPLTS(I) Node number for which the plot data are saved for post processing.

Examples:

```
PLOTS 1 3 2 writes plot file at every target time, and time
7 11 history at nodes 7, and 11.
Velocity is printed at node centers and interfaces.
```

```
PLOTS 10 0 2 writes plot file at every tenth time step, and time
7 11 history at nodes 7 and 11. Velocity is not printed.
```

2.2.3.6 Beginning of Recurrent Data [RECUrrent]

Recurrent Data

Keyword: **RECUrrent**Required

This keyword has no associated data and signals the completion of all initialization data and the beginning of the recurrent data section. The simulator proceeds with initialization calculations upon encountering this keyword or the ENDS keyword. This keyword must be the last keyword in the initialization data set and the first keyword of the recurrent data set.

Read: RECUrrent

RECUrrent Keyword signaling the end of initialization data. The control will pass to Recurrent data after this keyword unless an ENDS keyword is encountered after this keyword.

2.2.3.7 Solution Method [SOLVe]

Recurrent Data

Keyword: **SOLVe**

Required

This keyword specifies the linear equation solver method and overrides the one designated by default or previously specified.

Read: SOLVe ISOLVE NEWTNMN NEWTNMX NORTH NITMAX LEVEL

SOLVe Keyword for designating matrix solver and iterations.

ISOLVE Flag for choosing solver.

= 1 Thomas Algorithm for one-dimensional problem. For such problems, this method is internally set and will override any other specified method. Since all dual continuum model systems are at least two-dimensional, this solver should not be used for such systems. If assigned, it will internally reset to ISOLVE = 3

= 2 Not available

= 3 WATSOLV (ILU factorization) with GMRES accelerator

= 4 WATSOLV (ILU factorization) with CGSTAB accelerator [see WATSOLV User's Guide for details (van der Kwaak, et al., 1995)]

NEWTNMN Minimum number of Newtonian iterations before a check on convergence is made (default = 2; for pure conduction or pure liquid problem, default = 1).

NEWTNMX Maximum number of Newtonian iteration for convergence. Time step will be cut and equations resolved if the iterations exceed NEWTNMX (default = 7; for pure conduction and pure liquid system, default = 1).

NORTH Maximum number of vectors for orthogonalization for WATSOLV. Used only if ISOLVE = 3 (GMRES), (default = 4).

NITMAX Number of inner iterations for WATSOLV (default = 100).

LEVEL Degree of fill in incomplete LU factorization for WATSOLV, (default = 1).

Example:

```

:      isolve newtnmn newton north nitmax level
SOLVE 3      2      0      3      75      2

```

In this example, WATSOLV solver using GMRES with three orthogonalization vectors will be used. The level of fill is declared as two with two minimum Newtonian iterations and default value for maximum Newtonian iterations.

2.2.3.8 Source/Sink [SOURce]

Recurrent Data

Keyword: **SOURce**

Conditional

This keyword assigns a set of tables for sources and sinks as functions of time.

Read: SOURce NS SCALH SCALM FN

Unstructured Grid Read: M1 M2 INC ISTYPE

Structured Grid Read: IS1 IS2 JS1 JS2 KS1 KS2 ISTYPE

Read: TIMEQ QHT QMT

...
...
*

SOURce Keyword for assigning source/sink table.

NS Total number of sources and sinks.

FN File name from which the time varying source and sink data are read (optional). The file name must have an extension of `.src` in lowercase letters, but the extension should not be included in FN specification. The file name FN (excluding the extension) should not exceed six characters. The run will stop if the file name is misspelled or the file `fn.src` does not exist. (default = blank space, in which case the data are read from the input file).

M1, M2 Beginning and ending block numbers.

INC Increment of block numbers. Source will be assigned to all blocks from M1 to M2 in the increment of INC. (Default = 1).

IS1, IS2 Indices bounding the source/sink region in I-direction.

JS1, JS2 J directions.

KS1, KS2 K directions.

ISTYPE Index for type of source/sink, a two digit number denoted by *ij* where

- i = 1** mass of water
- i = 2** mass of air (not available yet)
- i = 3** heat source with no mass
- j = 1** rate for each grid block in the region [J/s]
- j = 2** rate per unit volume from which the total strength is computed based on block pore volume for the mass source and the bulk block volume for the heat source [J/m³/s]. For the dual continuum model, the heat strength is computed based on the block volume of the matrix continuum only and not the composite volume of the matrix and the fracture in the block
- j = 3** rate for the total specified region that is internally allocated to individual grid blocks based on pore volume for the mass and the bulk volume of blocks for the heat [J/s]

SCALH Scale factor or multiplier to read in values of QHT.

SCALM Scale factor or multiplier to read in values of QMT.

TIMEQ Time in seconds.

QHT = **Temperature** [°C], if ISTYPE = 1j or 2j (j = 1, 2, 3)
 = **Heat Rate** if ISTYPE = 3j (j = 1, 2, 3)

QMT = **Mass Rate** if ISTYPE = 1j or 2j (j = 1, 2, 3)
 = **0** if ISTYPE = 3j (j = 1, 2, 3)

The units for QHT are J/sec for j = 1 and 3, and J/m³/s for j = 2. The units for QMT are kg/s for j = 1 and 3, and kg/m³/s for j = 2.

The read in values for fluid and energy withdrawal must be negative (sink) and injection is positive (source). If QMT is specified as a negative value corresponding to a sink, QHT is not used. If QMT is a positive value corresponding to a mass source and QHT is read as a negative value, it will be interpreted as specific enthalpy rather than temperature. The code will compute enthalpy for a given temperature for the water phase. If 2-phase or steam is to be injected, directly read the enthalpy (as a negative value for input variable QHT).

Read TIMEQ, QHT, and QMT on one line successively in ascending order of TIMEQ. The desired time range is terminated by reading a line with slash (/), asterisks (*), or period (.) in column 1.

As simulation proceeds, source and sink rates are linearly interpolated from this table corresponding to the midpoint of the time step size. If a single entry is specified, a constant heat or mass source sink will be used. If simulation time exceeds the final entered time in the table, the last table entry will be used.

This completes data for one source.

Repeat the above sequence starting with reading IS1, IS2, etc. for the next source until all NS sources are specified. The number of entries or the time interval in each table (if more than one table) need not be the same.

In this release of METRA, source/sinks are assigned only to the matrix continuum for a dual continuum model system, while they are assigned to the fracture continuum for a multiple interacting continuum system.

Example:

Source 3 .5 0. !read-in heat source will be multiplied by .5

: i1 i2 j1 j2 k1 k2 istype

1 2 1 1 1 2 32

heat source per unit volume is specified in the region.

: time qh/vol

0. 1.3

1.e7 1.2

5.e8 .9

/

: i1 i2 j1 j2 k1 k2 istype

5 8 1 1 1 2 31

a uniform heat source is specified for each block

: time qh/blk 0 10. grid block 3.e7 7. 3.e9 5

/

: i1 i2 j1 j2 k1 k2 istyp

1 7 2 2 1 1 33

total heat source specified for the region

: time qh for the region 0 50. which is allocated to individual grid blocks

1.e7 40 proportional to the bulk volume for the blocks. 1.e8 30 1.e9 20 1.e10

10 0

2.2.3.9 Steady State [STEADy]

 Recurrent Data
Keyword: **STEADy**

Conditional

This keyword sets the run in a mode such that it will proceed marching in time until a steady state is reached. The steady state is determined based on a maximum saturation change, maximum temperature change, and maximum pressure change per year as set by the user with this keyword. Upon attaining the steady state, the time and the time step numbers are internally reinitialized to zero and new recurrent data sets may be read. The run may be terminated with an ENDS keyword following this keyword if only steady-state distribution is to be achieved.

Read: STEADy DPSTDY DSSTDY DTMPSDY

STEADy[u] Keyword for designating the run to march in time until a steady state is reached. The variable [u] in the bracket sets the units for time for monitoring the steps. See the keyword TIME for details on [u].

DPSTDY Maximum pressure rate of change to define a steady state [Pa/time unit] (default = 1.e-6).

DSSTDY Maximum saturation rate of change (default = 1.e-5).

DTMPSDY Maximum temperature rate of change [T/time unit] (default = 1.e-4).

Once the simulation proceeds up to a time when the absolute value of the maximum pressure change in any block divided by the time step in years is less than DPSTDY, the run will process the remaining data.

Examples:

```
STEADy [y]  1.e-6 1.e-5 1.e-8
```

The run will march in time until the maximum change per year in any block is less than 1.e-6 Pa/y for pressure, less than 1.e-5 1/y for saturation, and less than 1.e-8°C/y for temperature. These values are problem dependent and may need to be refined by trial and error.

2.2.3.10 Target Times [TIME]

Recurrent Data

Keyword: **TIME**

Required

This keyword sets the target times. Plot/graphic files are written when the simulation reaches a target time. Recurrent data may also be modified if desired. Recurrent data initially specified will remain in effect unless modified. New recurrent data sets not defined earlier may also be introduced at any time during a run.

A set of data between two target times is referred to as one set of recurrent data.

Read: TIME TTARGET DTT

TIME[u] Keyword for time step specifications. The variable [u] in the bracket sets the units for the target time and the time step size.

units of time	variable [u]
years	[y], [yr], [yrs], or [years]
months	[m], [mo], [mos], or [months]
days	[d], [day], or [days]
seconds	[s], [sec], or [secs]

The units of the target time and the time step size may be changed as often as desired by specifying different units for the variable [u] on subsequent TIME keywords. If an inadmissible value for [u] is specified, or no value is specified for it, the time defaults to seconds. Note that TIME[u] is treated as a single keyword, and as such there should not be any embedded blanks.

Unlike other Recurrent Data, the units for the target time must be set with each target time. Not assigning the units will default to the units of seconds.

The time for plot files will use the units of time as specified here.

TTARGET Target time up to which simulation will proceed. If read as a negative value, simulation will proceed $\text{abs}(\text{TTARGET})$ steps beyond this and stop, ignoring all subsequent input data. The units of the target time is as declared by the variable [u] in the keyword.

IF METRA is run in coupled mode with GEM, TTARGET is overridden by the variable TPLOT in GEM (see section describing GEM for details).

DTT > 0 Fixed time step size of magnitude DTT.
= 0 Compute internally

Examples:

```
Time          1000. 100.  ! (time in the units of second by default)
Time[sec]     1000. 100.  ! (time in the units of seconds)
Time[yr]      1.      .02  ! (time in the units of years)
```

Time[s], Time[d], Time[m], Time[y], etc., are acceptable keywords for specifying times in seconds, days, months, and years.

2.2.3.11 Convergence Tolerances [TOLR]

Recurrent Data

Keyword: **TOLR**

Optional

This keyword overrides or modifies the tolerances for convergence. If one or more of the tolerances are read as zero, it is internally set to its respective default value.

Read: TOLR TOLP TOLS TOLT TOLP2 TOLM TOLA TOLE RTWOTOL
RMXTOL SMXTOL

- TOLR** Keyword for assigning tolerances.
- TOLP** Pressure tolerance [Pa] (default = 10 Pa).
- TOLS** Saturation tolerance (default = 0.0001).
- TOLT** Temperature tolerance [°C] (default = 0.001).
- TOLP2** Air partial pressure tolerance [Pa] (default = 10 Pa).
- TOLM** Tolerance on mass residual (L2 error norm) (default = 1.e-5).
- TOLA** Tolerance on air residual (L2 error norm) (default = 0.001).
- TOLE** Tolerance on energy residual (L2 error norm) (default = 0.001).
- RTWOTOL** Initial residual norm (default = 1.e-7).
- RMXTOL** Absolute value of residual (default = 1.e-7).
- SMXTOL** Max of (dx, dx/x), where x = solution vector (default = 1.e-7).

For pure conduction and liquid options, the last three tolerances for WATSOLV default to 1.e-12 (refer to the WATSOLV User's Guide for details).

Residual (L2) = Max abs(Ax-b) for total mass, air, and energy equations = [abs(Ax-b)/Mass or energy] for each block.

2.2.4 Auxiliary Keywords

The keywords DEBUg, ENDS, MONItor, and RSTArt are auxiliary keywords which control the data flow and provide for monitoring and debugging.

2.2.4.1 Debug Output For Initialization [DEBUg]

Auxiliary

Keyword: DEBUg

Optional

This keyword prints out intermediate variables for a designated region of grid blocks for debugging or examination of intermediate results. This option should not be used for routine production runs because of the extensive output it produces.

Read: DEBUg IBUG

Unstructured Grid Read: M1 M2 INC

...
...
/

Structured Grid Read: I1 I2 J1 J2 K1 K2

...
...
/

DEBUg Keyword for printing intermediate variables.

IBUG Index designating the level or extent of output.

- = 0 Turn off the previously set debug output
- = 1 Print minimum amount of debug output
- = 2 Print intermediate level of debug output
- = 3 Print full debug output

M1, M2 Beginning and ending node numbers.

INC Increment of node numbers. Debug output will be printed for nodes M1 to M2 in increments of INC (default = 1).

I1, I2, J1, J2, K1, K2 Indices bounding the region in $x(r)$ -, $y(\theta)$ -, and z -directions for which more detailed output will be printed.

Comment(s):

Read one region per line and terminate the read-sequence by reading a slash (/), asterisk (*), or period (.) in column 1. Overlapping specification of regions will not cause any error, with last entry taking precedence. The DEBUg option is turned off internally upon completion of initialization. A new DEBUg keyword must be introduced for debug output in the recurrent-data section.

Example:

```
Debug 1          ! Level = 1
1 3 1 1 1 5     ! Region 1 for debug output
5 9 1 1 7 11    ! Region 2 for debug output
/               ! Debug region terminator (must be the last line)
```

2.2.4.2 Run Terminator [ENDS]

Auxiliary

Keyword: **ENDS**

Required

This keyword signals completion of a run. To complete initialization only, ENDS should be the last keyword in the initialization data set. For any run with time stepping, the ENDS keyword should be the last keyword of the recurrent data.

Read: ENDS

ENDS Keyword terminating run.

Example:

Ends! No data will be processed after this keyword.

2.2.4.3 Monitoring Nodes [MONitor]

 Auxiliary
Keyword: **MONitor**

Optional

The keyword **MONitor** allows monitoring key variables of designated nodes as a function of time. The information is written in the file `fn_prn`, which may be monitored as the simulation proceeds. This ASCII file may also be used to generate time-history plots at the monitored nodes.

Read: MONitor m1 m2 m3 m4 m5

MONitor Keyword for assigning elements to be monitored.

m1 . . . m5 Element numbers that are to be monitored. A maximum of five elements may be assigned.

An element number is calculated using the following relation:

$$m = i + (j - 1) nx + (k - 1) nx*ny \quad (2-5)$$

where i , j , and k are indices for a three-dimensional grid and m is the element number.

Example:

```
Monitor
1 3 7
```

Primary variables for these three nodes will be written in file `1fn_prn` at each time step.

2.2.4.4 Restart Options [RSTArt]

Recurrent Data

Keyword: **RSTArt**Optional

This keyword designates the frequency of writing restart plot files.

Read: RSTArt IRST1

RSTArt Keyword for reading restart/graphic files output.

IRST1 Frequency of writing cut-and-paste data.
= 0 Cut-and-paste data not written
n>0 Frequency in number of target times for writing cut-and-paste data
n<0 Frequency in number of time steps for writing cut-and-paste data

A cut-and-paste file can be extracted from `lfn_out` and cut and pasted into an initial run. The file is written in the required format for INIT data.

Examples:

```
RSTArt 10 ! writes a cut-and-paste data set at every tenth target time  
RSTArt -100 ! Writes a cut-and-paste data set at every 100th time step
```

2.3 GEM Input Data Keywords

2.3.1 Title Lines

Two title lines are required and must appear as the first two lines in the data file. Any alphanumeric characters may appear in the title with up to 80 characters per line. Blank lines may also appear in the title lines, but not in other keywords unless required. Comment lines [lines beginning with a colon (:)] can precede the title lines.

2.3.2 Input Data Keywords

There are currently 32 keywords used in the GEM input file. Appearing in alphabetical order, they are

Keyword	Status	Brief Description
AQCX	Optional	List of aqueous secondary species
AQIR	Optional	Kinetic data for homogeneous aqueous reactions
BCON	Required	Specify boundary conditions
BRKP	Optional	Specify nodes for time-history plot
COMPONENTS	Required	List of primary species and chemical compositions
CONSERVE	Optional	Conservation constraints for inlet or initial fluid
COUPLE	Optional	Coupling parameters with METRA
DBASE	Required	Specify thermodynamic database
DCMPARAMETERS	Optional*	Parameters for dual continuum model
DIFF	Required	Diffusion coefficients and tortuosity
DTSTEP	Required	Time step size control
DXYZ	Required*	Grid spacing
ENDS	Required	Marks end of input file (last keyword)
FLOW	Required*	Gas and liquid flow velocities
GASES	Optional	List of gaseous species
GRID	Required	Defines system geometry (first keyword)
IONX	Optional	List of ion-exchange species
ISYSTEM	Required	Specify if system is nonisothermal and partially saturated
MASTER	Optional	Species to control time stepping
MNIR	Optional	Kinetic reaction data for minerals
MNRL	Optional	List of minerals
NOSKIP	Optional	End skipping lines in input file
OPTS	Required	Various options
PLTFILES	Optional	Plotting options
PTINIT	Optional	Pressure-temperature profiles
SKIP	Optional	Begin skipping lines in input file

Keyword	Status	Brief Description
SOLVe	Required	Solver parameters
SOURce	Optional	Specification of source/sink
STOL	Optional	Tolerances for individual species
TIME	Required	Time printouts
TOLR	Optional	Tolerances for controlling time step
VOLUme	Optional*	Assign volumes and porosities to specified nodes

*Data for these keywords are overwritten by METRA in a coupled run.

Each keyword is described in detail in alphabetical order in the following sections. The order of appearance of the keywords in the input file is generally arbitrary with the exception of certain keywords which must appear in the proper sequence. The GRID keyword must be the first keyword, and the ENDS keyword is the last keyword. Keywords BCON and SOURce must not appear before the COMPONENTS keyword.

2.3.2.1 Aqueous Secondary Species [AQCX]

Initialization Data

Keyword: **AQCX**

Optional

This keyword reads in the names of aqueous secondary species as defined by the chemical reactions as written in Eq. (B-1). In the absence of secondary species, this keyword is not required.

Read: AQCX**Read:** SPECIES DIFFUSION

AQCX Keyword for reading in a list of aqueous secondary species and their diffusion coefficients. For the case $IDIF \geq 1$ (see DIFF keyword) their corresponding diffusion coefficients are also read in.

SPECIES Name of species.

DIFFUSION Aqueous diffusion coefficient for corresponding species [cm^2/s]. For $IDIF = 0$, these values are ignored. If $IDIF > 0$ and a zero value for DIFFUSION is read in, then the value of DO read from the DIFF keyword is used.

Comment(s):

Species-dependent diffusion coefficients are only possible with $IDIF \geq 1$.

The name of the species must agree with the name entered in the databases, `master25.V8.R5` or `mastertemp.V8.R5`, or any other database the user provides.

For each secondary species there must be corresponding primary or other secondary species for the stoichiometric reaction coefficients and equilibrium constant to be loaded from the thermodynamic database. It is left to the user to decide which species are to be included as secondary species. The only restriction is that the primary species must form an independent set. Thus, either H^+ or OH^- may be chosen as primary species. The remaining species must appear in the list of secondary species. Likewise, if $\text{Al}(\text{OH})_4^-$ is chosen as a primary species, Al^{3+} must appear as a secondary species.

The list of species is terminated with a slash (/), asterisk (*), or period (.) in column 1.

Example:

```
AQCX
: species      coef.
  oh-          5e-5
  aloh+2       0e-5
  al(oh)2+     0e-5
  al(oh)3(aq)  0e-5
  al(oh)4-     0e-5
  h3sio4-      0e-5
  h2sio4-2     0e-5
:blank
```

2.3.2.2 Kinetic (Irreversible) Homogeneous Aqueous Reactions [AQIR]

Initialization Data

Keyword: **AQIR**

Optional

The keyword reads in the names of irreversibly reacting aqueous species and associated kinetic reaction rate data as defined in Eq. (B-33). This includes the type of reaction, kinetic rate constant, transport limited rate, surface area, and others. The reaction may be either homogeneous or heterogeneous but may not involve the electron as the aqueous species.

Read:	AQIR
Read:	SPECIES NBXNAQ DELHAQ
Read:	ITYPKINAQ NPRIAQ NSECAQ RKAQ
Read:	SPECIES SKAQ
AQIR	Keyword for reading in kinetic reaction data for minerals.
SPECIES	Name of aqueous species. The aqueous species must correspond to the last species listed in the COMPONENT keyword.
NRXNAQ	Number of linearly dependent parallel reaction. NRXN = 1 for a single reaction mechanism.
DELHAQ	Activation enthalpy of reaction [kJ/mole].
ITYPKINAQ	Type of reaction. = 20 Transition state rate law [see Eq. (B-33)] = 25 Transport limited transition state rate law [see Eq. (B-34)]
NPRIAQ	Number of primary species in prefactor [see Eq. (B-26)].
NSECAQ	Number of secondary species in prefactor [see Eq. (B-26)].
RKAQ	Rate constant [moles/cm ² /s].
SPECIES	Species name.
SKAQ	Rate coefficient.

Comment(s):

Each species name must also appear at the end of the COMPONENT keyword and must agree with the name appearing in the thermodynamic database. A negative value for the rate constant implies logarithm to the base 10.

The entire block ends with a slash (/), asterisk (*), or period (.) in column 1.

Example:

```
AQIR
: species  npar  delhag  [kj/mole]
O2(aq)      1      40.
:itypkaq   npri  nsec  rk  [moles/cm3/s]
   30      1      0  1.0e-10
O2(aq)      1.0
:
h2(aq)      1      20
   30      1      1.02e-10
h+ 0.753507
/
/
```

2.3.2.3 Boundary Conditions [BCON]

Initialization Data

Keyword: **BCON**

Required

This keyword reads in the boundary condition data for defining the composition of a multicomponent fluid. In this version of the code, only concentration, zero flux, and zero gradient boundary conditions are possible. Zero flux is the default boundary condition. The boundary condition is applied uniformly over the specified region of the face of the bounding surface. For a structure grid the boundary surface consists of one of the faces of a rectangular parallelepiped, or the faces of the bounding cylinder in cylindrical coordinates. The origin of coordinates for Cartesian coordinates is taken in the upper left corner of the parallelepiped at the front face with the z-axis pointing downward, the y-axis horizontal, and the x-axis perpendicular to the yz-plane forming a left-handed coordinate system (see Figure 2-2). For the case of cylindrical geometry, the origin is at the top, centered on the axis of the cylinder.

Read: BCON

Read: IBNDTYP IFACE TMPBC DIST AREA VELL VELG POR SL PORM SLM
IMTX

Unstructured Grid Read: M1 M2 INC

Structured Grid Read: I1 I2 J1 J2 K1 K2

Read: SPECIES ITYPE CTOT CONSPEC GUESS

Dual Continuum Model Matrix Read: SPECIES ITYPE CTOT CONSPEC GUESS

BCON Keyword for specifying boundary conditions.

IBNDTYP Type of boundary condition.

- = 1 Concentration boundary condition
- = 2 Not used
- = 3 Zero gradient boundary condition (no diffusive flux)

IFACE Boundary at which solution composition is to be determined (see figure 2-2).

IFACE is not used for unstructured grid.

- = 1 Left face or inner radius in cylindrical coordinates ($I = 1, X = 0$)
- = 2 Right face or outer radius in cylindrical coordinates ($I = NX$)

= 3	Top face (K = 1, Z = 0)
= 4	Bottom face (K = NZ)
= 5	Front face (J = 1, Y = 0)
= 6	Back face (J = NY)
TMPBC	Temperature at designated surface [°C]
DIST	Distance from boundary to block center [m] (default value = $\frac{1}{2} \Delta x$, $\frac{1}{2} \Delta y$, or $\frac{1}{2} \Delta z$ depending on IFACE for the structured grid, and d_i for the unstructured grid).
AREA	Area of block surface over which boundary condition is imposed [m ²] (default value = Δy , Δz , $\Delta x \Delta z$ or $\Delta x \Delta y$ for the structured grid area between nodes connecting I1 and I2 for the unstructured grid).
VELL	Liquid velocity at boundary [m/s] (default = VLX0 read by keyword FLOW or as specified by METRA in a coupled node).
VELG	Gas velocity at boundary [m/s] (same as liquid velocity).
POR	Porosity at boundary (default = porosity of the boundary block).
SL	Liquid saturation at boundary (default = liquid saturation of the boundary block).
PORM	Matrix porosity at boundary (default = matrix porosity of the boundary block).
SLM	Matrix saturation at boundary (default = matrix saturation of the boundary block).
IMTX	Parameter to determine matrix flux in dual continuum model option.
= 0	Use IBNDTYP for matrix boundary condition
= 1	Zero flux matrix boundary condition
M1, M2	Beginning and ending connected node numbers in increments of INC.
INC	Node increment.
I1, I2	Indices specifying region in the I-direction.
J1, J2	Indices specifying region in the J-direction.
K1, K2	Indices specifying region in the K-direction.
SPECIES	Name of a primary species.

ITYPE Type of constraint condition imposed on species mass balance equation.

- = -1 Charge balance constraint
- = 1 Total concentration as specified by CTOT
- = 3 Mineral constraining species
- = 4 Gaseous constraining species
- = 7 Individual species concentration as specified by CTOT
- = 8 Solution pH as specified by CTOT
- = 10 Conserved quantity determined from titration substances specified by the keyword CONSERve

CTOT Total concentration (ITYPE = 1), species concentration (ITYPE = 7), gas partial pressure (ITYPE = 4), or pH (ITYPE = 8) depending on ITYPE. This field is not used for ITYPE = 3, or -1. A negative value for CTOT implies logarithm to the base 10.

CONSPEC Name of mineral or gaseous species with which the solution is to be in equilibrium.

GUESS Initial guess for primary species concentrations [molality]. If not specified, guess is computed internally.

Comment(s):

Default is to impose zero-flux boundary conditions on all faces.

Names of primary species must be listed in the same order in keywords BCON, COMPONENTS, and SOURCE and spelling must be identical to the names appearing in the thermodynamic database. The BCON keyword must come after the COMPONENTS keyword in its input file.

In a coupled run, the number and type of boundary conditions and the region over which they are specified must agree with the BCON specifications in METRA. In this case the variables TMPBC, DIST, VELL, VELG, POR, SL, PORM, and SLM are set from METRA.

Multiple lines of input may be used to specify the boundary region. The condition applies to the union of the specified regions. The node specification block must end with a slash (/), asterisk (*), or period (.) in column 1. Each block of data specified over a region must end with a slash (/), asterisk (*), or period (.) in column 1.

If a constraint mineral or gaseous species is not used, the CONSPEC field may be left blank unless a guess is specified in which case a blank (' ') must be inserted.

For the dual continuum model, separate boundary fluid composition data are read in for fracture and matrix continua, in that order.

Example:

```
BCON
:ibndtyp iface tmpbc dist area vl vg porbnd slbnd porbndm slbndm ibndmtx
  1          1
:il  i2  j1  J2  K1  k2
  1  1  1  1  1  1
/
:species itype ctot      mineral/gas      guess
k+       1      1.e-6
al+3     1      1.e-8
h+       8      4.0
sio2(aq) 1      1.e-6
/
```

2.3.2.4 Break-Through Node Points for Plotting [BRKP]

Initialization Data

Keyword: **BRKP**

Optional

This keyword is for reading a list of blocks at which solution composition data is stored at each time step for producing time-history plots.

Read: BRKP NDXMAX

Read: IDX(I), JDY(J), KDZ (K)

BRKP Keyword for reading block at which data is stored as a function of time.

NDXMAX Number of block points to be read in.

Comment(s):

There is one entry per line, with a maximum of 50 entries.

The block positions for a structured grid are given as the integer triplet (IDX JDY KDZ).

The indices IDX, JDY, and KDZ refer to a particular block point:

$NDX = IDX + (JDY - 1) * NX + (KDZ - 1) * NX * NY$

Example:

```
BRKP 5
1 1 93
1 1 110
1 1 130
1 1 150
1 1 185
```

2.3.2.5 Initial Conditions and Definition of Component Species [COMPONENTS]

Initialization Data

Keyword: **COMPONENTS**

Required

This is the keyword for defining the initial conditions and specification of primary (component) species that are used to define the chemical system. Each input composition specification must be preceded by specification of the region over which the solution composition is to apply. The COMPONENTS keyword must precede the keywords BCON and SOURCE in the input file.

Read: COMPONENTS

Unstructured Grid Read: M1 M2 INC

Structured Grid Read: I1 I2 J1 J2 K1 K2

Read: SPECIES ITYPE CTOT CONSPEC GUESS

Dual Continuum Model Matrix Read: SPECIES ITYPE CTOT CONSPEC GUESS

COMPONENTS Keyword for assigning system primary species, initial concentrations, and diffusion coefficients.

M1, M2 Beginning and ending connected node numbers in increments of INC.

INC Node increment.

I1, I2 Indices specifying region in the I-direction.

J1, J2 Indices specifying region in the J-direction.

K1, K2 Indices specifying region in the K-direction.

SPECIES Name of primary species.

ITYPE Type of constraint condition imposed on species mass balance equation.

- = -1 Charge balance constraint
- = 1 Total concentration as specified by CTOT
- = 3 Mineral constraining species

- = 4 Gaseous constraining species (gas partial pressure = CTOT)
- = 7 Individual species concentration as specified by CTOT
- = 8 Solution pH as specified by CTOT
- = 10 Conserved quantity determined from titrated substances specified by the keyword CONSeRve

CTOT Total concentration (ITYPE = 1), species concentration (ITYPE = 7), gas partial pressure (ITYPE = 4), or pH (ITYPE = 8) depending on ITYPE. This field is not used for ITYPE = 3, or -1. A negative value for CTOT implies logarithm to the base 10.

CONSPEc Name of mineral or gaseous species with which the solution is to be in equilibrium.

GUESS Initial guess for primary species concentration [molality]. If not specified the initial guess is computed internally.

Comment(s):

Multiple input lines may be used to specify the region. The block ends with a slash (/), asterisk (*), or period (.) in column 1. The complete list of initial conditions ends with a slash (/), asterisk (*), or period (.) in column 1. The maximum number of regions is set by the parameter NREG located in the `paramtrs.h` file.

The order in which primary species are entered in the input file must be the same for the BCON and COMPONENTS keywords and spelling must be identical to the names appearing in the thermodynamic database.

For an isothermal system, the initial conditions are applied uniformly over each region specified. For a nonisothermal system, speciation is carried out at each block using the specified initial temperature and the composition specification assigned to the region in which the node resides.

If a constraint mineral or gaseous species is not used, the CONSPEc field may be left blank unless a guess is specified, in which case a blank ("") must be inserted.

The input variable GUESS is used to provide an initial guess to the Newton-Raphson iteration scheme used to solve for the distribution of species. The variable GUESS is not used if a numeral or gas constraint is specified.

For the dual continuum model, separate initial fluid composition data are read in for fracture and matrix continua in that order.

Example: Single continuum with uniform initial conditions.

```

COMPONENTS
:      I1      I2      J1      J2      K1      K2
      1      100     1       1       1       1
/
: species  itype   ctot   mineral/gas  guess
k+         3       1.e-4  k-feldspar
al+3       3       1.e-4  muscovite
h+         8       7.0
sio2(aq)   3       1.e-3  quartz
hco3-      4       -2      co2(g)
/

```

Example: Single continuum with nonuniform initial conditions. The second set of conditions overwrites the first.

```

COMPONENTS
:      I1      I2      J1      J2      K1      K2
      1      100     1       1       1       1
/
: species  itype   ctot   mineral/gas  guess
k+         3       1.e-4  k-feldspar
al+3       3       1.e-4  muscovite
h+         8       7.0
sio2(aq)   3       1.e-3  quartz
hco3-      4       -2      co2(g)
      51      70     1       1       1       1
/
: species  itype   ctot   mineral/gas  guess
k+         3       1.e-4  k-feldspar
al+3       3       1.e-4  muscovite
h+         8       6.0
sio2(aq)   3       1.e-3  quartz
hco3-      4       -2      co2(g)
/
/

```

Example: Single continuum with nonuniform initial conditions. This example is equivalent to the previous.

```

COMPONENTS
:      I1      I2      J1      J2      K1      K2
      1      50     1       1       1       1
      71      100     1       1       1       1
/
: species  itype   ctot   mineral/gas  guess
k+         3       1.e-4  k-feldspar
al+3       3       1.e-4  muscovite
h+         8       7.0
sio2(aq)   3       1.e-3  quartz
hco3-      4       -2      co2(g)
      51      70     1       1       1       1
/
/

```

```

: species  itype  ctot  mineral/gas  guess
k+         3      1.e-4  k-feldspar   k-feldspar
al+3      3      1.e-4  muscovite    muscovite
h+        8      6.0    quartz       quartz
sio2(aq)  3      1.e-3  quartz       quartz
hco3-     4      -2     co2(g)       co2(g)
/
/

```

Example: Dual-continuum with uniform initial conditions. Initial conditions for fractures are read first, then matrix.

```

COMPONENTS
:   I1   I2   J1   J2   K1   K2
   1   100  1    1    1    1
/
: species  itype  ctot  mineral/gas  guess
k+         3      1.e-4  k-feldspar   k-feldspar
al+3      3      1.e-4  muscovite    muscovite
h+        8      7.0    quartz       quartz
sio2(aq)  3      1.e-3  quartz       quartz
hco3-     4      -2     co2(g)       co2(g)
/
k+         3      1.e-4  k-feldspar   k-feldspar
al+3      3      1.e-4  muscovite    muscovite
h+        8      7.0    quartz       quartz
sio2(aq)  3      1.e-3  uartz        uartz
hco3-     4      -2     co2(g)       co2(g)
/

```

2.3.2.6 Option for Computing Conserved Quantities [CONServe]

Initialization Data

Keyword: **CONServe**Optional

This keyword is used to construct conserved quantities during titration of a set of substances into pure water. The conserved quantities may be used as constraints (itype = 10) in constructing the initial (keyword COMP) and boundary (keyword BCON) fluid compositions.

Read: CONServe

Read: NAME

CONServe Keyword to read in titration substances used to construct conserved quantities.

NAME Name of substance (aqueous or mineral species).

Comment(s):

The number of conserved quantities is equal to the number of primary species minus the number of titration substances.

Example:

```
CONServe  
hno3 (aq)  
fe (oh) 3  
fes2
```

2.3.2.7 Coupling METRA and GEM [COUPl_e]

 Initialization Data
Keyword: **COUPl_e**

Optional

This keyword defines parameters to invoke coupling of porosity and permeability and enables synchronization of time steps between METRA and GEM.

Read: COUPl_e ISYNC IPOR IPERM PERMFAC PORFAC ICKSAT SLCUTOFF

COUPl_e Keyword for coupling changes in porosity and permeability and synchronizing time stepping between METRA and GEM.

ISYNC Parameter for synchronizing time steps with MULTIFLO.

- = **n** Integer defining fraction of METRA time step attempted by GEM
- = **0** A value of zero implies no synchronization

IPOR Parameter for invoking variable porosity

- = **0** Constant porosity
- = **1** Variable porosity

IPERM Parameter for invoking variable permeability.

- = **0** Constant permeability
- = **1** Variable permeability

PERMFAC Exponent n in permeability/porosity expression [see Eq. (B-37) in Appendix B].

PORFAC Exponent n in porosity dependence of tortuosity [see Eq. (B-38) in Appendix B].

ICKSAT Activate check for saturation below minimum specified by parameter SLCUTOFF.

SLCUTOFF Minimum liquid saturation allowed in two-phase flow calculation with METRA coupled to GEM (icode = 3 or 4) or GEM in stand alone mode (icon = 2). If saturation goes below this value, velocities and transmissibilities for both gas and liquid phases are set to zero in GEM until the saturation rises above the cutoff value. The saturation cutoff does not affect the saturation computed by METRA.

Comment(s):

The parameter ISYNC should only be nonzero when running GEM in implicit mode.

Example:

```
      :      isync  ipor  iperm  permfac  porfor  
COUPlE 4      1      1      3.      1.
```

2.3.2.8 Thermodynamic Database File [DBASe]

Initialization Data

Keyword: **DBASe**

Required

This keyword assigns the thermodynamic database for reading chemical reactions for homogeneous and heterogeneous reactions involving minerals, aqueous, and gaseous species.

Read: DBASe

Read: DATABASE

DATABASE Name of thermodynamic database including path on UNIX system.

Example:

/home/skippy/lichtner/bin/database/mastertemp.V8.R5

2.3.2.9 Dual Continuum Model Parameters [DCMParameters]

Initialization Data

Keyword: **DCMParameters**

Required for dual continuum model formulation

This keyword defines parameters used to invoke the dual continuum model formulation.

Read: DCMParameters

Unstructured Grid Read: M1 M2 INC SIGMAF AREAMOD XLM YLM ZLM PORM,
SWM

Structured Grid Read: I1 I2 J1 J2 K1 K2 SIGMAF AREAMOD XLM YLM ZLM,
PORM, SWM

M1, M2 Beginning and ending node numbers.

INC Increment of node numbers. Default value of INC = 1.

I1, I2, J1, J2, K1, K2 Indices bounding the region in x (r)-, y (θ)-, and z -directions for which more detailed output will be printed.

SIGMAF Fraction of volume occupied by fractures in the defined region.

AREAMOD Factor by which internally computed matrix-fracture interface areas to be multiplied. The matrix-fracture area is computed by the relations given in Subsection A.6. Note that a value of zero for AREAMOD will decouple the matrix and fracture continua.

XLM, YLM, ZLM Average size of matrix blocks in x -, y -, and z -directions. If the fracture spacing is large corresponding to large matrix blocks in a given direction, the corresponding values of XLM, YLM, or ZLM may be set to zero, in which case the internally computed matrix-fracture surface area will be ignored in that direction.

PORM Matrix porosity fraction

SWM Matrix liquid saturation fraction

Comment(s):

Read one region per line and terminate the read sequence by reading a slash (/), asterisk (*), or period (.) in column 1. Overlapping specification of regions will not cause any error, with last entry taking precedence.

Example:

```
DCMParameters  
1 3 1 1 1 5 0.01 1. .1 .1 .1  
/
```

2.3.2.10 Aqueous and Gaseous Diffusion [DIFF]

 Initialization Data
Keyword: **DIFF**

Required

 This keyword assigns aqueous and gaseous diffusion coefficients and tortuosities.
Read: DIFF D0 DELHAQ DGAS DGEXP TORTAQ TORTG IDIF**DIFF** Keyword for reading diffusion coefficient data for aqueous and gaseous species.**D0** Aqueous diffusion coefficient [cm²/s].**DELHAQ** Activation enthalpy [kJ/mol].**DGAS** Gaseous diffusion coefficient [see Eq. (A-16)] [cm²/s].**DGEXP** Exponent in expression for gaseous diffusion coefficient [see Eq. (A-16)].**TORTAQ** Tortuosity factor for aqueous diffusion.**TORTG** Tortuosity factor for gaseous diffusion.**IDIF** Parameter to specify species-dependent or species-independent aqueous diffusion coefficients and corrosion model (default = 0).

= 0 Species-independent aqueous diffusion coefficients

= 1 Species-dependent aqueous diffusion coefficients

= 2 Corrosion model

= 3 Corrosion model

If IDIF ≥ 1

Read: SPECIES DIFAQ

Aqueous diffusion coefficients for primary species [cm²/s]. This field is used only if IDIF ≥ 1 on the DIFF keyword. Any number of species may be listed in any order. If a primary species appearing in the COMP keyword is not listed here, then the diffusion coefficient defined by the variable D0 is used.

SPECIES Name of the primary species**DIFAQ** Diffusion coefficient for the species "SPECIES"

Example:

```
: d0[cm2/s] delhaq[kJ/mol] dgas[cm2/s] dgexp tortaq tortg idif
DIFF 1.d-5 12.6 2.13d-1 1.8 1.d0 1.d0 0
: species diffusion coef [cm2/s]
cs+ 2.1e-5
cu+ 1.2e-5
h+ 0.312e-5
k+ 1.957e-5
na+ 1.334e-5
nh4+ 1.954e-5
f- 2.1e-5
cl- 2.032e-5
hco3- 60.e-6
hso4- 1.33e-5
i- 2.044e-5
oh- 5.26e-5
cu+2 0.8e-5
ca+2 0.792e-5
fe+2 0.8e-5
mg+2 0.706e-5
ni+2 0.8e-5
sr+2 0.9e-5
zn+2 0.8e-5
so4-2 1.065e-5
o2(aq) 2.09e-5
h2(aq) 2.09e-5
/
```

2.3.2.11 Initial and Maximum Time Step [DTSTep]

Initialization Data

Keyword: **DTSTep**

Required

This keyword assigns the initial time step for the run and the maximum allowed time step within a specified time interval.

Read: DTSTep[u] NSTPMAX (TSTEP(I), I = 1, NSTPMAX)

Read: (DT (I), I = 1, NSTPMAX+1)

DTSTep[u] Keyword for specifying the initial and maximum time steps within a prescribed time interval. The variable [u] in brackets allows different units to be chosen for the target time and time step, defined

units of time	variable [u]
years	[y], [Y]
days	[d], [D]
minutes	[m], [M]
hours	[h], [H]
seconds	[s], [S]

The keyword DTSTep[u] is treated as a single keyword without any blank spaces.

NSTPMAX Number of time intervals for which the maximum time step is specified.

TSTEP Times at which maximum time step is changed [u].

DT Maximum time step size [u] for time interval [TSTEP(I-1), TSTEP (I)] for I = 1, ..., NSTPMAX, with TSTEP(0) = 0.

Comment(s):

In implicit mode, DT[NSTPMAX+1] represents the largest possible time step. In operator-splitting and explicit modes, DT[NSTPMAX+1] represents the time step once the system has reached a stationary state. DT[1] in all cases represents the initial time step.

Example:

```
DTST[y]  1 3.e-8  
1.e-8    1.e2
```

In this example, the maximum time step is 10^{-8} yr for three steps. After 3×10^{-8} yr, the maximum time step is 100 yr. The initial time step is 1×10^{-8} yr. It is desirable to begin a calculation with a sufficiently small time step so that initially a reduction in step size does not take place.

2.3.2.12 Grid-Block Sizes [DXYZ]

Initialization Data

Keyword: **DXYZ**

Conditional

This keyword designates the size of grid blocks in $x(r)$ -, $y(\theta)$ -, and z -directions. It also specifies the choice of grid as to block-centered (default) or point-distributed (not implemented). This data set may be omitted if the grid block coordinates are specified with the keyword CXYZ or if UNSTRUCTURED grid geometry is used. For an unstructured grid, data associated with this dataset are ignored.

Read: DXYZ IGRID RW RE

Read: (DX(I), I = 1, NX)

Read: (DY(J), J = 1, NY)

Read: (DZ(K), K = 1, NZ)

DXYZ Keyword for reading grid-block sizes.

IGRID Index for grid-type.

= 0 block centered

= 1 Point-Distributed (not implemented)

= 2 Boundary node at the surface corresponding to CTOUGH (Nitao, 1989)

RW Inner boundary radius for cylindrical system [m].

RE Outer boundary radius for cylindrical system [m].
For Cartesian geometry, RW and RE are not required, and ignored if specified.

DX Block sizes in x -direction [m]. For a cylindrical system, DX designates the radius to block center from the axis of the cylinder.

DY Block sizes in y -direction [m]. For a cylindrical system, DY designates the sector angle of a block in degrees.

DZ Block thicknesses [m]. Note that the z -direction is positive downward with the top block numbered as 1 and the bottom block as NZ.

Comment(s):

For cylindrical geometry, fewer than NX nonzero values for DX may be read, in which case the rest will be computed internally based on logarithmic spacing. The inner radius RW must satisfy the inequality $RW < DX(1)$.

Values are read in order of DX, DY, and DZ starting DX, DY, and DZ each on a new line. Read NX nonzero values for DX, NY values for DY, and NZ values for DZ. In any case, whether DX(), DY(), and DZ() are zero or not, exactly NX, NY, and NZ values, respectively, must be read for DX(), DY(), and DZ().

For an unstructured grid, NX, NY, and NZ as read by the GRID keyword are not used for internal computations. However, values for DX, DY, and DZ are still read in corresponding to the values specified for NX, NY, and NZ in the GRID keyword. If either NX, NY, or NZ is zero, no value for DX, DY, or DZ may be read.

Examples:

Cartesian Geometry:

```

      igrid  rw  re
DXYZ  0      0  0
: dx(1) dx(2)....
1. 1. 1.5 1.5 2. 2. 3. 3. 5. 10.! x-direction
15. 15. 40.
: dy(1)
1.                                ! y-direction
: dz(1) dz(2) ...
10. 20. 30. 45. 60. 50. 50. 150.! z-direction

```

This example, designates block sizes for a Cartesian grid system of 13 blocks in the x-direction, 1 block in the y-direction, and 8 blocks in the z-direction.

Cylindrical Geometry:

```

: igrid      rw  re
DXYZ  0      .001 100. ! radial geometry with inner and outer radius of
:                                cylinder .001 and 100 m.
:
:      r(1)  r(2)
:      .5    1.    11*0. ! only 2 values are specified. The rest will be
:                                computed internally.
:
: dy(1)
90.                                ! one angular sector of 90 degrees.
: dz(1)      dz(2) ...
10. 20. 30. 10. 20. 40. 100. 150.! z-direction

```

2.3.2.13 End of Run [ENDS]

Initialization Data

Keyword: **ENDS**

Required

This keyword terminates the run and must be the last keyword in the input file.

Read: ENDS

ENDS Keyword terminating run.

Any data appearing after this keyword is not processed and remains intact in the input file.

Example:

```
: end of input file  
Ends
```

2.3.2.14 Liquid and Gas Flow Velocities and Dispersivity [FLOW]

Initialization Data

Keyword: **FLOW**

Required

This keyword defines flow parameters for stand-alone mode of GEM. For icode = 3 and 4, the values for the velocities are taken from METRA.

Read: FLOW VLX0 VLY0 VLZ0 VGX0 VGY0 VGZ0 ALPHAX ALPHAY ALPHAZ
VMFAC

FLOW Keyword for defining flow field.

VLX0 Liquid flow velocity in the I-direction [m/y].

VLY0 Liquid flow velocity in the J-direction [m/y].

VLZ0 Liquid flow velocity in the K-direction [m/y].

VGX0 Gas flow velocities in the I-direction [m/y].

VGY0 Gas flow velocities in the J-direction [m/y].

VGZ0 Gas flow velocities in the K-direction [m/y].

ALPHAX Dispersion length in the I-direction [m]. (Not implemented)

ALPHAY Dispersion length in the J-direction [m]. (Not implemented)

ALPHAZ Dispersion length in the K-direction [m]. (Not implemented)

VMFAC Fraction of flow (matrix to fracture velocity ratio) taking place in matrix in dual continuum model option, fraction.

Comment(s):

The Courant number is only used to control the time step size for the operator-splitting and explicit algorithms.

Example:

```

:      vlx0    vly0    vlz0    vgx0    vgz0 [m/yr]  alphax  alphay  alphaz [m]  vmfac
FLOW  1.      0.      0.      0.      0.          0.      0.      0.

```

2.3.2.15 Gaseous Species [GASEs]

Initialization Data

Keyword: **GASEs**Optional

This keyword reads in the names of gases. This keyword is not needed if there are no gaseous species.

Read: GASEs**Read:** NAME**GASEs** Keyword for reading in the names of gaseous species.**NAME** Name of gaseous species.

Comment(s):

The names of gaseous species must be identical to the corresponding names read from the thermodynamic database file. One species is read per line. The data block is terminated with a slash (/), asterisk (*), or period (.) in column 1.

Example:

```
GASEs  
co2 (g)  
O2 (g)  
/
```

2.3.2.16 Grid Geometry [GRID]

Initialization Data

Keyword: **GRID**

Required

The GRID keyword defines the grid geometry (radial, Cartesian, or unstructured), dual continuum model or single continuum, number of nodes in each direction, and other optional parameters.

Read: GRID GEOMETRY NX NY NZ IFREQ IPRINT IWARN IDEBUG IDBG1 IDBG2

GRID Keyword defining grid geometry and optional parameters.

GEOMETRY Coordinate system geometry.

- = **RADIAL** Cylindrical geometry
- = **XYZ** Cartesian geometry
- = **UNSTRUCTURED** Unstructured grid
- = **DCMRAD** Dual continuum model formulation with cylindrical geometry
- = **DCMXYZ** Dual continuum model formulation with Cartesian geometry
- = **DCMUNSTRUCTURED** Dual continuum model formulation with unstructured grid

NX Number of grid blocks in x or r (I) direction.

NY Number of grid blocks in y (J) direction (for a radial system, NY = 1).

NZ Number of grid blocks in z (K) direction.

IFREQ Number of time steps between screen output.

IPRINT Parameter for printout control.

- = -1 Minimum printout
- = 0 Small printout
- = 1 Intermediate printout
- = 2 Maximum printout
- = 3 Database printout

IWARN Parameter for controlling warning messages.

- = 0 No warning messages (default)
- = 1 Print level 1 warning messages
- = 2 Print level 2 warning messages
- = 3 Print level 3 warning messages

IDEBUG Parameter for obtaining debugging printout.

- = 0 No debugging printout (default)
- = 1 Minimum debug printout in output file (mostly initialization)
- = 2 Intermediate debug output (initialization and intermediate concentrations)
- = 3 Full debug output (This option produces large amounts of output, including matrices passed to WATSOLV)

IDBG1, IDBG2 Range of nodes for debug printout.

Comment(s):

This keyword must appear as the first keyword in the input file.

Problems for one-, two-, and three-dimensional are defined by appropriate assignment of NX, NY, and NZ. Maximum number of grid blocks in any direction and the total number of blocks permissible can be altered by the user in the `paramtrs.h` file.

For the unstructured grid option. NX, NY, and NZ are not used.

Example:

```
: geometry nx ny nz ifreq iprint iwarn idebug ibg1 ibg2
GRID XYZ 100 1 100 2 -1
```

2.3.2.17 Ion-Exchange Reactions [IONX]

Initialization Data

Keyword: **IONX**

Optional

Keyword for reading input data for ion-exchange reactions as defined by the chemical reactions Eq. (B-4).

Read: IONX NEX CEC

Read: (SELEX(I)=1,NEX)

IONX Keyword for reading ion-exchange data.

NEX Number of cations participating in ion-exchange reactions.

CEC Cation exchange capacity [see Eq. (B-19)] [moles/L].

SELEX Selectivity coefficient K_{jk} [see Eq. (B-18)]. NEX values are to be read in with up to 10 entries per line.

Comment(s):

Cations involved in ion-exchange reactions must appear first in the list of primary species in the BCON and COMPONENTS keywords and in the same order as the selectivity coefficients. The selectivity coefficients correspond to the exchange reactions as written in Eq. (B-4).

Example:

```

:      ion-exchange  reactions
IONX  8 0.035
: na+    k+    ca+2  mg+2  cu+2  al+3  fe+2
  1.00   5.00  2.50  3.98  3.98  4.68  2.75

```

In this example, the cation exchange capacity is 0.035 moles. The selectivity coefficients are derived from Table 1 in Appelo (1996), referenced to sodium with unit selectivity coefficient.

2.3.2.18 System Parameters [ISYSstem]

Initialization Data

Keyword: **ISYSstem**

Required

This keyword defines whether the system is isothermal or nonisothermal and reads in values for the porosity and saturation as well as other parameters.

Read: ISYSstem ISAT ISOTHRM IREAD POR0 PHIR SAT W LAMBDA TOLDELT
TOLPOR

ISYSstem Keyword for assigning system parameters.

ISAT Parameter for designating number of phases in system.

- = -1 Pure liquid system
- = 0 Two-phase liquid-gas system

ISOTHRM Parameter for assigning system temperature dependence.

- = 0 Isothermal system
- = 1 Nonisothermal system

IREAD Index for reading the velocity field or saturation from external files.

- = 0 Do not read input data or compute permeability field
- = 1 Read x-y-stochastic velocity fields from files `xvelocity` and `yvelocity` with the binary format


```
open(3, file='xvelocity', form='unformatted', status='old')
open(4, file='yvelocity', form='unformatted', status='old')
read(3) ((vlx(ix+(iy-1)*nxp1),ix=1,nxp1),iy=1,ny)
read(4) ((vly(ix+(iy-1)*nx),ix=1,nx),iy=1,nyp1)
```
- = 2 Read from binary files with the same name as in 1 with the format


```
open(3, file='xvelocity', status='old')
open(4, file='yvelocity', status='old')
read(3,*) ((vlx(ix+(iy-1)*nxp1),ix=1,nxp1),iy=1,ny)
read(4,*) ((vly(ix+(iy-1)*nx), ix=1,nx),iy=1,nyp1)
```

- = 4 Read saturation profile from file sat.dat with the format

```
read(3,*,err = 333) ltitle
do n = 1, nmax
read(3,*) xx,sat0(n) for one-dimensional problems
read(3,*) xx,yy,sat0(n) for two-dimensional problems
enddo
```
- = 5 Read density, temperature, and velocity fields computed from METRA (not implemented)

PORO Initial porosity if constant. Not used in coupled mode.

PHIR Initial reacting volume fraction.

SAT Initial saturation of liquid phase. Not used in coupled mode.

W Spatial averaging factor (not implemented).

LAMBDA Time-weighting factor in the implicit finite difference algorithm.

TOLDELT Zone boundary tolerance (not implemented).

TOLPOR Minimum allowed porosity. If the porosity becomes lower than this value due to mineral precipitation, it is set equal to this value.

Example:

```

:          isat  isothrm  iread  por0  phir  sat  w  lambda  toldelt  tolpor
ISYSstem  0      1          0    .1    1.   0.5 .5   1.     1.e-3   1.e-3

```

This example applies to a two-phase, nonisothermal system. The values specified for W and TOLDELT are ignored.

2.3.2.19 Setting Master Species For Time Step Control [MASTer]

Initialization Data

Keyword: **MASTer**

Optional

This keyword defines the master species for controlling the time step size.

Read: MASTer MASPEC

MASTer Keyword for specifying master species.

MASPEC Name of primary species for controlling time step size. Specifying ALL implies all primary species are used (default = ALL).

Example:

```
:master species for controlling time stepping  
MASTer h+
```

2.3.2.20 Kinetic (Irreversible) Mineral Reactions [MNIR]

Initialization Data

Keyword: **MNIR**

Optional

This keyword reads in the names of irreversibly reacting minerals and associated kinetic reaction rate data as defined in Eqs. (B-25) and (B-28). This includes the type of reaction, kinetic rate constant, initial volume fraction, surface area, and others.

Read: MNIR**Read:** MINERAL NRXN FKIN DELH TAU**Read:** ITYPKIN NPRI NSEC SIG RK**Read:** SPECIES SK**Unstructured Grid Read:** M1 M2 INC PHI AREA PHIF AREAF**Structured Grid Read:** I1 I2 J1 J2 K1 K2 PHI AREA PHIF AREAF**MNIR** Keyword for reading in kinetic reaction data for mineral.**MINERAL** Name of mineral.**NRXN** Number of linearly dependent parallel reactions NRXN = 1 for a single reaction mechanism.**FKIN** Degree of supersaturation required before mineral can precipitate.**DELH** Activation enthalpy of reaction [kJ/mole].**TAU** Tolerance for allowed maximum change in mineral volume fraction over a time step.**ITYPKIN** Type of reaction.

= 20 Transition state rate law [see Eq. (B-25)]

= 25 Transport-limited transition state rate law [see Eq. (B-28)]

NPRI Number of primary species in prefactor [see Eq. (B-26)].**NSEC** Number of secondary species in prefactor. [see Eq. (B-26)].

- SIG** Tempkin constant [see Eq. (B-25)].
- RK** Rate constant [moles/cm²/s].
- SPECIES** Species name.
- SK** Rate coefficient.
- M1, M2** Beginning and ending node numbers.
- INC** Increment of node numbers.
- I1, I2, J1, J2, K1, K2** Specification of region for structured grid.
- INC** Node increment for unstructured grid.
- PHI** Initial volume fraction in specified region. For the dual continuum model option, PHI refers to matrix volume fraction.
- AREA** Initial specific mineral surface area in specified region [see Eq. (B-25)] [1/cm]. For the dual continuum model option, AREA refers to matrix surface area.
- PHIF** Initial fracture volume fraction in specified region for dual continuum model option.
- AREAF** Initial fracture specific mineral surface area in specified region [see Eq. (B-25)] for dual continuum model option [1/cm].

Comment(s):

Each mineral name must also appear in the MNRL keyword and must agree with the name appearing in the thermodynamic database. A negative value for the rate constant (RK) implies logarithm to the base 10.

Any number of region specifications are allowed for a given mineral, but the entire computational domain must be covered. A slash (/), asterisk (*), or period (.) in column 1 ends the region specification. If two regions overlap, the last data read in applies. The maximum number of minerals that can be read in is specified by the parameter `nkmax` located in the `paramtrs.h` file.

The entire block ends with a slash (/), asterisk (*), or period (.) in column 1.

Example:

```

MNIR
:mineral  nrxn  fkin  delh  tau
k-feldspar  1    1.   35.   1.e-3
: itypkin  npri  nsec  sig  rk
   20      0    0    1    3.02e-3
:
:         matrix  fracture
:i1 i2 j1 j2 k1 k2 vol  area  vol  area
1 200  1 1  1 1  0.2  6.0    0    60.
/
gibbsite  1  1    35.  1.e-3
   20      0  0    1   -14.
1 200  1 1  1 1  0.0    1.    0.0  1.
/
kaolinite  1  1.  35.  1.e-3
: itypkin  npri  nsec  sig  rk
   20      0    0    1   -14
1 200  1 1  1 1  0.0    1  0.0  1.
/
muscovite  1  1.  35.  1.  -14

: itypkin  npri  nsec  sig  rk
   20      0    0    1   -14.
1 200  1 1  1 1  0.0    1.    0.0  1
/
quartz  1  1.  35.  1.e-3
: itypkin  npri  nsec  sig  rk
   20      0    0    1.  3.16e-18
1 200  1 1 1 1  0.75 60    0.  60.
/
/

```

2.3.2.21 Mineral Species [MNRL]

Initialization Data

Keyword: **MNRL**Optional

This keyword reads in the names of minerals.

Read: MNRL**Read:** NAME**MNRL** Keyword to read in the names of minerals.**NAME** Name of mineral. The mineral name must agree with the entry in the thermodynamic database.**Comment(s):**

The list of minerals is terminated by a slash (/), asterisk (*), or period (.) in column 1.

Example:

```
MNRL
quartz
kaolinite
k-feldspar
muscovite
gibbsite
: /
```

2.3.2.22 Various Parameters and Options [OPTS]

Initialization Data

Keyword: **OPTS**

Required

This keyword defines various numerical options and parameters.

Read: OPTS METHOD IOPS IFOR IFLXLIM ITMAX IHALMAX NDTCMX LOGLIN
ISTEPDT

Read: ISURF IACT ISST WTUP COURNR DTCUTF DELCMX QKMAX WTKIN TPULSE

OPTS Keyword for defining time-stepping and spatial differencing options and parameters.

METHOD Parameter for selecting implicit, operator-splitting, or explicit time stepping algorithm.

- = 1 Implicit time stepping algorithm
- = 2 Operator splitting
- = 3 Explicit time stepping algorithm

IOPS Parameter for selecting operator-splitting algorithm. Used if METHOD = 2.

- = 0 Operator-splitting algorithm with explicit liquid transport. Gas phase is always treated implicitly.
- = 1 Operator-splitting algorithm with all phases implicit
- = 2 Operator-splitting algorithm: Strang's formulation

IFOR Parameter for selecting spatial finite differencing.

- = 0 Hybrid
- = 1 Central finite difference
- = 2 First order upwinding
- = 3 First order upwinding with a specified weight factor (WTUP)
- = 4 Total Variation Diminishing algorithm

IFLXLIM Parameter for selecting flux-limiter in Total Variation Diminishing algorithm. Used if IFOR = 4.

- = 0 Leonard flux limiter
- = 1 Van Leer flux limiter
- = 2 Fromm limiter
- = 3 minmod limiter

- ITMAX** Maximum number of Newton-Raphson iterations in a time step.
- IHALMAX** Maximum number of time step cuts.
- NDTCMX** Number of steps with constant step size Δt following a time step cut.
- LOGLIN** Parameter for selecting concentration variable.
- = 0 Use logarithm of concentrations (recommended)
 - = 1 Do not use logarithms
- ISTEPDT** Parameter for controlling time step adjustment
- = 1 Use global rate of change of concentration (uses **TTOL**, pg. 2-122).
 - = 2 Use number of iterations to control time step (recommended).
 - = 3 Use maximum change in concentration (**DELTCMX**) to control.
- IBCOS** Parameter for including boundary condition in reactive step of operator splitting algorithm. It is used only for IOPS = 1.
- = 0 Do not include boundary condition in reactive step.
 - = 1 Do include boundary condition in reactive step.
- ISURF** Parameter for computing changes in mineral surface area.
- = 0 Constant surface area
 - = 1 Evolving surface area
- IACT** Parameter for selecting activity coefficient algorithm.
- = 0 Do not compute activity coefficients
 - = 1 Compute activity coefficients
- ISST** Option for choosing stationary state time integration.
- = -1 Do not use stationary state integration
 - = 1 Use stationary state integration (use with caution)
- WTUP** Weighting factor for upstream weighting. Used only for IFOR = 3.
- COURNR** Courant number used to limit time step for explicit transport.
- DTCUTF** Time-step reduction factor following a time-step failure (default = 0.5).

DELCMX Concentration change for automatic time-step algorithm.

QKMAX Maximum activity product change in log formulation (default = 500).

WTKIN Weighting factor for reactions in operator-splitting algorithm (default = 0.5).

TPULSE Time at which inlet concentration is set to initial concentration. This option is used to generate a concentration pulse in the inlet field.

Comment(s):

The operator splitting mode (METHOD = 2) greatly reduces the run time for problems involving a large number of chemical components. The implicit (IOPS = 1) and explicit (IOPS = 0) options apply to the transport step in the operator-splitting algorithm. The second step involving chemical reactions is always done implicitly.

The higher-order Total Variation Diminishing algorithm (IFOR = 4) allows advection-dominated transport to be modeled with reduced numerical dispersion. It can be used with implicit or explicit treatment of the transport.

The preferred spatial finite difference algorithm for implicit transport (METHOD = 1 or METHOD = 2, IOPS = 2) is the hybrid scheme IFOR = 0. With this option, the difference scheme is tuned adaptively between the central and upstream weighting.

The Courant number is used to limit the size of the allowable time step. For the fully implicit time stepping algorithm and the implicit-transport variant of the operator-splitting algorithm, the Courant number may be greater than one. Taking the Courant number too large may result in excessive time truncation errors. If transport is treated explicitly, the Courant number must be less than one. Limitation of the time step by the Courant number applies only to the transient solution and is not invoked when the system reaches a stationary state.

Example: Fully implicit time-stepping algorithm with hybrid spatial differencing.

```

:      method  iops  ifor  iflxlim  itmax  ihalmx  ndtcmx  loglin  istepdt
OPTS   1      0    0      0      32     16     1      0      2
:  isurf  iact  isst  wtup  cournr  dtcutf  delcmax  qkmax  wtkin  tpulse
      1      0    -1     0     5e2    .50    0.05    500

```

Example: Operator-splitting algorithm with implicit transport and hybrid spatial differencing.

```

:      method  iops  ifor  iflxlim  itmax  ihalmx  ndtcmx  loglin  istepdt
OPTS   2      1    0      0      32     16     1      0      2
:  isurf  iact  isst  wtup  cournr  dtcutf  delcmax  qkmax  wtkin  tpulse
      1      0    -1     0     5e2    .50    0.05    500

```

2.3.2.23 Writing Plot Files [PLTFiles]

Initialization Data

Keyword: **PLTFiles**

Optional

This keyword determines which plot files are to be produced during the run. A zero indicates no plot file is written.

Read: PLTFiles**Read:** IPLOT A S T M SI SF V Z B IN E EX TI G ITEX MK ERR VE**IPLOT** Parameter to determine if plot files should be created.

= 0 No plot file written (default = 0)

= 1 Plot file written

A Aqueous primary species.**S** Secondary species.**T** Total concentrations.**M** Mineral reaction rates.**SI** Saturation indices.**SF** Surface area.**V** Mineral volume fractions.**Z** Mineral zone boundary positions.**B** Breakthrough curve.

= 1 Primary species concentrations

= 2 Total primary species concentrations

= 3 Primary and secondary species concentrations

IN Time-dependent inlet fluid composition (not implemented).

- E** Electrical potential.
- EX** Ion-exchange solid concentration.
- TI** Not used.
- G** Gaseous species concentrations.
- ITEX** Table format parameter.
- = 1 Generate LaTeX (e.g., Goossens, et al., 1994) formatted table of inlet fluid composition for use in word processing
- = 2 ASCII formatted table
- MK** Monode kinetics.
- ERR** Mass balance errors.
- VE** Electrochemical migration velocities.

Example:

```

      PLTFiles
:iplot  a  s  t  m  si  sf  v  z  b  in  e  ex  ti  g  itex  mk  err  ve
        1  1  1  1  0  0  1  0  0  0  0  0  0  1  0  0  1  0

```

2.3.2.24 Initial Temperature and Pressure [PTINit]

Initialization Data

Keyword: **PTINit**

Optional

This keyword defines initial temperature and pressure for standalone mode. In coupled mode (*icode* = 3 or 4), the temperature and pressure are provided by METRA.

Read: PTINit P(Pa) TEMP IFLGTMP A B C D X0 XLEN

PTINit Keyword for reading in initial temperature and pressure.

P Initial pressure [bars] (default = 1 bar).

TEMP Initial temperature [°C] (default = 25°C).

IFLGTMP Flag for specifying temperature profile.

- = 0** Constant temperature
- = 1** $T(X) = D X^3 + A X^2 + B X + C$
- = 2** $T(X) = A + (B-A) \text{EXP}[-((X-X_0)/C)^2] + (D-A) * X / XLEN$
- = 3** $T(X,T) = A + \frac{1}{2}(B-A) (\text{ERF}[(X+C-X_0)/(2\text{SQRT}(DT))] - \text{ERF}[(X-C-X_0)/(2\text{SQRT}(DT))])$

A, B, C, D, X0, XLEN Parameters used in temperature profile.

Example:

:	p (Pa)	temp	flag	a	b	c	d	x0	xlen
PINit	1.e5	25.	0	25	300	250	125	1000.	2.d3

2.3.2.25 Method of Solution [SOLVe]

Initialization Data

Keyword: **SOLVe**

Required

This keyword specifies the method of solution as the WATSOLV conjugate gradient solver or a tri-diagonal solver for one-dimensional problems.

Read: SOLVe ISOLV LEVEL NORTH NITMAX IDetail RMAXTOL RTWOTOL
SMAXTOL TOLEXP

SOLVe Keyword for specifying the matrix solver.

ISOLVE Flag to choose solver.

- = 1 Tri-diagonal solver
- = 2 Not used
- = 3 WATSOLV (ILU factorization) with GMRES accelerator
- = 4 WATSOLV (ILU factorization) with CGSTAB accelerator

LEVEL Degree of fill in incomplete LU factorization for WATSOLV (default = 1).

NORTH Maximum number of vectors used for orthogonalization in WATSOLV. Used only if ISOLVE = 3 (GMRES) (default = 4).

NITMAX Maximum number of inner iterations for WATSOLV (default = 100).

IDetail Debugging option

- = 0 Do not print debug output
- = 1 Print compressed matrix and incomplete factorized matrix coefficients.

RMAXTOL Absolute value of residual (default = 1.e-12).

RTWOTOL WATSOLV tolerance parameter.

SMAXTOL Maximum of $|dx, dx/x|$, where x = solution vector (default = 1.e-12).

Comment(s):

For further details on use of the WATSOLV conjugate gradient solver, see the WATSOLV User's Manual (van der Kwaak, et al., 1995).

Example:

```
:  isolv  level  northn  itmax  idetail  rmax  tol    rtwotol  smaxtol
SOLV   3      1      1      0      0    1.e-20 1.e-20  1.e-12
```

2.3.2.26 Source/Sink [SOURce]

Initialization Data

Keyword: **SOURce**

Optional

This keyword assigns sources and sinks as a function of time at specified blocks. This keyword must not appear before its COMPONents keyword in the input file.

Read: SOURce NS SCALE

Unstructured Grid Read: MS1, MS2, INC, (IDUM, I = 1,3), ISTYPE

Structured Grid Read: IS1 IS2 JS1 JS2 KS1 KS2 ISTYPE

Read: TIMEQ TEMPQ QM
 ...
 ...
 0

If QMT > 0 Read: SPECIES ITYPE CTOT CONSPEC GUESS

SOURce Keyword for assigning source/sink.

NS Total number of source and sink.

SCALE Scale factor that multiplies QM.

IS1, IS2 Indices defining the source/sink region in I-direction.

JS1, JS2 Indices defining the source/sink region in J-direction.

KS1, KS2 Indices defining the source/sink region in K-direction.

ISTYPE Index for the type of source/sink specified as a two digit number of the form ij.

i = 1 mass of water
i = 2 mass of air (not implemented)
j = 1 rate for each grid block in the assigned region
j = 2 rate per unit volume (not implemented)
j = 3 rate for total specified region (not implemented)

TIMEQ	Time in seconds.
TEMPQ	Temperature [°C].
QMT	Mass rate [kg/s].
SPECIES	Name of a primary species.
ITYPE	Type of constraint condition imposed on species mass balance equation. <ul style="list-style-type: none"> = -1 Charge balance constraint = 1 Total concentration as specified by CTOT = 3 Mineral constraining species = 4 Gaseous constraining species = 7 Individual species concentration as specified by CTOT = 8 Solution pH as specified by CTOT = 10 Conserved quantity determined from titration substances specified by the keyword CONSeRve
CTOT	Total concentration, species concentration, or pH depending on the value of ITYPE. This field is not used for ITYPE = 3, 4, or -1. A negative value for CTOT implies logarithm to the base 10.
CONSPEc	Name of mineral or gaseous species with which the solution is to be in equilibrium.
GUESS	Initial guess for primary species concentrations [molality]. If not specified, the guess is computed internally.

Comment(s):

Names of primary species must be listed in the same order as in keywords BCON and COMPOnents and spelling must be identical to the names appearing in the thermodynamic database.

The source/sink block must end with a slash (/), asterisk (*), or period (.) in column 1. Each block of data specified over a region must end with a slash (/), asterisk (*), or period (.) in column 1.

If a constraint mineral or gaseous species is not used, the CONSPEc field may be left blank.

The source/sink is specified for matrix continuum for the dual continuum model option.

Example:

```
: ns scalm
SOURCE 2 0.0082
: is js ks istyp
  1 1 1 1 1 1 11
: timeq(sec) T/qht (oC/(J/s)) qmt (kg/s)
  .0      25.0      6.31e-1
0
: is js ks istyp
  25 25 25 25 1 1 11
: timeq(sec) T/qht (oC/(J/s)) qmt (kg/s)
  .0      25.0     -6.31e-1
0
```

2.3.2.27 Relative Tolerances [STOL]

Initialization Data

Keyword: **STOL**

Optional

This keyword reads in relative tolerances for primary species.

Read: STOL (ATOL(I), I = 1, NCOMP)

STOL Keyword for reading relative tolerances.

ATOL Relative primary species tolerances (maximum 10 per line) (default = 1).

Example:

```
STOL 1. 1. 1. 1. 1. 1. 1.
```

2.3.2.28 Target Time [TIME]

Initialization Data

Keyword: **TIME**

Required

This keyword reads the target times at which plot files and output of the run are produced.

Read: TIME NPRIN (TPLOT(I), I = 1,NPRIN)

TIME Keyword for specifying the target time.

NPRIN Number of target times specified with the same units [u] as specified in the DTStep keyword.

TPLOT Target times. Up to nine entries are allowed on the first line and a maximum of 10 on succeeding lines.

Example:

```
TIME 4 2.5e4 5.e4 1.e5 2.e5
```

2.3.2.29 Convergence Tolerances [TOLR]

 Initialization Data

Keyword: TOLR

Required

This keyword reads various parameters to control tolerances determining convergence of the solution.

Read: TOLR TOL TTOL TOLNEG TOLPOS TOLSTDST TOLC

TOLR Keyword defining various tolerances.

TOL Convergence tolerance for the residuals (default = 1.e-10).

TTOL Time step accelerator (default = 1.e-3).

TOLNEG Maximum negative mineral volume fraction allowed (default = 1.e-3).

TOLPOS Minimum convergence tolerance used in computing aqueous solution compositions for initial and boundary conditions.

TOLSTDST Steady-state test for convergence [see discussion following Eq. (B-41)] (default = 1.e-6).

TOLC Convergence tolerance for the primary species concentrations (default = TOL).

Solution is considered converged if either $TOL > \text{Residual}$ or $TOLC \geq \max |C_i^{k+1} - C_i^k|$.

Comment(s):

For explicit transport algorithms, TTOL should be set to a value greater than one. For the implicit solution algorithm, TTOL should generally be less than one. The optimal value must be determined by experimentation to obtain the smallest run time.

Example:

```

:   tol      ttol  tolneg  tolpos  tolstdste  tolc
TOLR 1.d-10   2.e3  1.e0    0.      1.e-6      1.e-12

```

2.3.2.30 Node Volume [VOLUME]

Initialization Data

Keyword: **VOLUME**

Optional

This keyword assigns volumes and porosities to specified nodes overriding the volume computed from the grid spacing.

Unstructured Grid Read: M1 M2 INC UVB UPOR

Structured Grid Read: I1 I2 J1 J2 K1 K2 UVB UPOR

VOLU Keyword defining volume and porosity assignment.

M1, M2 Beginning and ending node numbers.

INC Increment of node numbers.

I1, I2, J1, J2, K1, K2 Region specification.

INC Increment for unstructured grid.

UVB Volume [m³].

UPOR Porosity.

Comment(s);

If either UPOR or UVB is zero, the values read in previously are used. In a coupled run, the volumes and porosities assigned by METRA are used.

Example:

```

:      I1   i2   j1   j2   k1   k2   vol   por
VOLU   1    1    1    1    1    10 1.e6   0.1

```

3 SAMPLE INPUT DATA

3.1 METRA Input File

The structure of the METRA input file is as follows:

```
Title           (2 lines)
RSTArt
GRID
DXYZ           (or CXYZ)
THERmal
PCKR
PHIK
INIT
RECUrrent-data
OUTPUt*
SOLVe
TOLR*
LIMIT*
AUTO*
BCON*
SOURce*
PLOTs*
TIME [ ]
STEAdy [ ]*
ENDS
```

All keywords are required with the exception of those marked with an asterisk (*).

3.1.1 METRA Sample Input File: Two-Dimensional Radial Geometry

This problem describes the thermal-hydrologic effects of emplacement of high-level waste in a partially saturated host rock such as the proposed repository at Yucca Mountain, Nevada. The following data set describes a two-dimensional radial system with a time-varying decaying heat source with an initial heat load of 83.4 MTU/acre placed at a depth of 225 m in a partially saturated host rock in two spatial dimensions. The waste is represented by a circular disk and cylindrical symmetry is assumed. An initial heat load of 114 kw/acre is used in the calculation. The equivalent continuum model is not used in this example. The matrix/fracture system is represented by the equivalent continuum model (Lichtner and Walton, 1994). Four stratigraphic units are included in the model: Tiva Canyon (0–100 m), Paintbrush (100–150 m), Topopah Spring (150–475 m), and Calico Hills (475–600 m). The system is initially in equilibrium with a temperature of 15 °C at the surface and 30 °C at the water table located at the bottom. Initial conditions are read from the file *init.int*. Dirichlet boundary conditions at the top and bottom are imposed using large volume blocks at these boundaries. No flow at the lateral boundaries is assumed. The system is discretized into 61 × 68 elements of varying thicknesses ranging from 1.0 to 25 m. The simulation run is set to proceed to 10,000 years.

Example:

Data for Multiflo simulator (initial data : 2D, 83.4 AML, Yucca Mt.)
May 1998

```

RSTART 0
:
: XYZ          = 1 table look-up, pref = ref. press.
: RADIAL      = 0 correlations,  tref = ref temp.
: OTHER
:grid geometry nx ny nz ivplwr ipvtab iout gravity pref tref href
Grid RADIAL   61 1  68 1      1      3  0      0  0  0
:
Pckr                      :relative perm and pc keyword
: i type-curv swirm rpmm(lamda) alpham swext sgc iecm
:          swirf rpfm(lamda) alphaf phim phif permm permf
:Tiva Canyon (0-100 m)
  1 Van-Gen  0.04  0.3600  8.4e-7  0.  0.      1
              0.04  0.7636  1.305e-5 0.087 1.8e-3 9.7e-19 3.9e-12
:Paintbrush (100-150 m)
  2 Van-Gen  0.10  0.8500  1.53e-6 0.  0.      1
              0.04  0.7636  1.305e-5 0.421 1.8e-3 3.9e-14 3.9e-13
:Topopah Spring (150-475 m)
  3 Van-Gen  0.08  0.4400  5.8e-7  0.  0.      1
              0.04  0.7636  1.305e-5 0.139 1.8e-3 1.9e-18 3.9e-12
:Calico Hills (475-600 m)
  4 Van-Gen  0.11  0.3800  3.13e-7 0.  0.  1
              0.04  0.7636  1.305e-5 0.306 1.8e-3 2.0e-18 3.9e-12
/
:
Thermal-prop
: no  rho      cpr      ckdry      cksat      crp      crt      tau      cdiff      cexp      enbd
  1  2.580e+  3 728.  1.69  1.69  0  0  .5  2.13e-5  1.8  0.
  2  2.580e+  3 422.  0.61  0.61  0  0  .5  2.13e-5  1.8  0.
  3  2.580e+  3 840.  2.10  2.10  0  0  .5  2.13e-5  1.8  0.
  4  2.580e+  3 526.  1.42  1.42  0  0  .5  2.13e-5  1.8  0.
/
:          igrd      rw      re
DXYZ      0          0.      1.5e3
: (dx(i),i=1,nx)
10.00  30.00  50.00  70.00  90.00  110.0  130.0  150.0  170.0  190.0
210.0  230.0  250.0  270.0  290.0  310.0  330.0  350.0  370.0  390.0
410.0  430.0  450.0  470.0  490.0  510.0  530.0  550.0  570.0  590.0
610.0  630.0  650.0  670.0  690.0  710.0  730.0  750.0  770.0  790.0
810.0  830.0  850.0  870.0  890.0  910.0  930.0  950.0  970.0  990.0
1010.  1030.  1050.  1070.  1090.  1125.  1175.  1225.  1275.  1350.
1450.
:
: (dy(j),j=1,ny)
360.
:

```

```

: (dz(k),k=1,nz)
25.00 25.00 25.00 25.00 25.00 25.00 25.00 25.00 25.00
25.00
25.00 25.00 10.00 5.000 5.000 5.000 5.000 2.000 2.000 2.000
2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000
2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000
2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000 2.000
2.000 2.000 5.000 5.000 5.000 5.000 5.000 5.000 5.000 5.000
10.00 10.00 15.00 25.00 25.00 25.00 25.00 25.00 25.00 25.00

```

PhiK

```

: il i2 j1 j2 k1 k2 iist ithrm vb porm permx permy
permz
1 61 1 1 1 4 1 1 0.
1 61 1 1 5 6 2 2 0.
1 61 1 1 7 63 3 3 0.
1 61 1 1 64 68 4 4 0.
/

```

Init init

```

: il i2 j1 j2 k1 k2 pm tm sgm x2m
: 1 61 1 1 1 68 1.e5 25.0 0.5 0.
:/

```

```

:
: EQUIL 587.50 1.e5 30. 0.0255319 0.0 -1
:

```

Recurrent-data

```

:
Bcon 2
:itype iface il i2 j1 j2
1 TOP 1 61 1 1
:time qbc pbc tbc sgbc xabc
0. 0. 8.55e4 15.0 0.2 0.
/

```

```

1 BOTTOM 1 61 1 1
0. 0. 9.05e4 30.0 0.0 0.
/

```

Rstart 1 0

```

Output A=1 C=1 B=1
: isolve newtnmn newtnmx north nitmx level
:Solve 3 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-12 1.e-12 1.e-12
:
:Limit dpmx dsmlx dtmpmx dp2mx dtmn dtmx dtfac
LIMIT 1.e4 .08 10. 1.e5 1.e-6 1.e3 .5
:Plots 1
:Steady[y] 1.e-8 1.e-6 1.e-3
:Ends
: ns fach facm (fach and facm are multipliers to
: read-in values of qht and qmt)

```

```

:Source 1 6. 79353e6 1.
Source 1 3.39676e6 1.
: is js ks istyp
1 52 1 1 40 40 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
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
/
Output  A=1  C=1
:
:RSTArt 0 1
:
:   isolve  newtnmn  newtnmx  north  nitmx  level
Solve  3      1      7      4      100   1
:
:AUTO-step  DPMXE    DSMXE    DTMPMXE  DP2MXe  TACCEL  IAUTO
AUTO-step  1.E+4    0.025  3.0      1.e4    1.e-2   0
:
:TOLR  TOLP    TOLS    TOLT  TOLP2  TOLM  TOLA  TOLE
Tolr  10.e+0  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  dtfac
LIMIT  5.e4    .05    5.      1.e5   1.e-6  1.e4  .5
Plots  1 1 1
2380
Time [y] 10.
Time [y] 100.
Time [y] 500.
Time [y] 1000.
Time [y] 5000.
Time [y] 10000.
Ends

```

3.2 GEM Sample Input Data: Two-Dimensional Repository Problem

The corresponding GEM input file for the repository problem is presented in Section 3.1.1 for coupled mode using the implicit finite difference algorithm of GEM (method = 1). To avoid complete dryout in the vicinity of the repository, a heat loading of 83.4 MTU/acre is used in the calculation for which compute dryout does not occur. No other modifications need be made to the METRA input file to run in coupled mode.

The GEM input file `masin` takes into account seven primary species: Na^+ , K^+ , Ca^{2+} , H^+ , HCO_3^- , SiO_2 , and Cl^- ; three minerals: quartz, calcite, and halite; two gaseous species: $\text{CO}_{2(g)}$ and $\text{O}_{2(g)}$; and a number of aqueous complexes. The initial fluid composition is derived from J-13 groundwater and the initial host rock is assumed to consist of pure quartz with 90 percent by volume and 10 percent porosity. The simulation is run to 2,000 years. Zero gradient boundary conditions are imposed at the top and bottom of the computational domain. The input file `masin` for this problem is as follows

```

Test Data for Multiflo Simulator (Yucca Mt., 2D, 83.4 kW/acre)
      May 1998
:
:   geometry nx ny nz ifreg iprint iwarn idebug
GRID  RADIAL 61 1 68 2 0 0 0
:

```

```

: method iops ifor iflxlim itmax ihalmx ndteq loglin istepdt
OPTS 2 0 0 0 32 16 1 0 2
: isurf iact isst wtup cournr dtcutf delcmax gkmax tpulse
1 0 -1 0 5e3 .50 0.05 500
:
: isys ipor iperm permfac porfac icksat slcutoff
COUple 0 0 0 3. 0. 1 0.01
:
PLTFiles
:iplot a s t m si sf v z b in e ex ti g itex
1 1 1 1 1 0 0 1 0 2 0 0 0 0 1 0
:
: tol ttol tolneg tolpos tolexp dthalf qkmax tolstdst tolc
TOLR 1.d-10 2.e-3 1.e0 1.e-2 5.d0 .5 590. 1.e-12 1.e-12
:
: mcyc cc c flx r sp qk pk rk a1 a2 a3
DEBUg 0 1 1 0 1 1 1 1 1
:
: isat isotherm iread por0 phir sat w lambda toldelt tolpor
ISYSstem 0 1 0 .10162 1. 0. 5 .5 1. 1.e-3 1.e-3
:
: vx0 vy0 vz0 vgx vgy vgz[m/yr] alphax alphay alphaz[m]
vmfac
FLOW 0. 0. 1. 0. 0. 0. 0. 0. 0.
:
: d0[cm2/s] delhaq[kJ/mol] dgas[cm2/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 x3 + a x2 + 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 (Pa) 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
61*1.
1.
68*1.
:
: isolv level north nitmax idetail rmaxtol rtwotol smaxtol
SOLV 4 1 1 100 0 1.e-20 1.e-20 1.e-12
:
:initial and boundary conditions: 1-conc., 2-flux, 3-zero gradient
COMP
:
: i1 i2 j1 j2 k1 k2
1 61 1 1 1 68
/

```

```

:species  itype  ctot  mineral/gas  guess
ca+2      3      2.5e-3  calcite
mg+2      1      7.8e-4
na+       1      3.0e-3
k+        1      3.6e-4
h+        -1     8.2
hco3-     4      -2.00   co2(g)
sio2(aq)  1      1.5e-3
cl-       1      2.8e-3
so4-2     1      1.7e-3
o2(aq)    4      0.2     o2(g)
/
/
:
BCON
1 3
:ibntyp  iface  tmpbc  dist  area  vl  g  porbnd  slbnd  porbndm  slbndm
ibndmtx
3      1      25.
:il      i2  j1  j2  k1  k2
1      1  1  1  1  68
/

:species  itype  ctot  mineral/guess  guess
ca+2      3      2.5e-3  calcite
mg+2      1      7.8e-4
na+       1      3.0e-3
k+        1      3.6e-4
h+        -1     8.2
hco3-     4      -2.00   co2(g)
sio2(aq)  1      1.5e-3
cl-       1      2.8e-3
so4-2     1      1.7e-3
o2(aq)    4  0.2     o2(g)
:
3  2  25
61 61 1  1  1  68
/

: species  itype  ctot  mineral  guess  guess
ca+2      3      2.5e-3  calcite
mg+2      1      7.8e-4
na+       1      3.0e-3
k+        1      3.6e-4
h+        -1     8.2
hco3-     4      -2.00   co2(g)
sio2(aq)  1      1.5e-3
cl-       1      2.8e-3
so4-2     1      1.7e-3
o2(aq)    4      0.2     o2(g)
:
1 3  25.
1 61 1  1  1  1
/

:species  itype  ctot  mineral  guess
ca+2      3      2.5e-3  calcite

```

```

mg+2      1      7.8e-4
na+       1      3.0e-3
k+        1      3.6e-4
h+        -1     8.2
hco3-     4      -2.00      co2 (g)
sio2(aq)  1      1.5e-3
cl-       1      2.8e-3
so4-2     1      1.7e-3
o2(aq)    4      0.2      o2 (g)
:
  1 4 25.
  1 61 1 1 68 68
/
:species  itype  ctot  mineral  guess
ca+2      3      2.5e-3  calcite
mg+2      1      7.8e-4
na+       1      3.0e-4
h+        -1     8.2
hc03-     4      -2.00   Co2(g)
sio2(aq)  1      1.5e-3
cl-       1      2.8e-3
so4-2     1      1.7e-3
o2(aq)    4      0.2    O2(g)
:
/
: 10 entries per line
STOL 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
:
AQCX
oh-
h2(aq)
hso4-
hcl(aq)
co2(aq)
co3-2
caco3(aq)
cahco3+
caoh+
cacl+
cacl2(aq)
caso4(aq)
mgoh+
mgco3(aq)
mgcl+
mgghco3+
mgso4(aq)
nahco3(aq)
nacl(aq)
naoh(aq)
naso4-
kcl(aq)
khso4(aq)
kso4-
h3sio4-

```

```

h2sio4-2
/
:
MNRL
calcite
/
:
GASEs
co2(g)
o2(g)
h2(g)
/
MNIR
:mineral npar fkin delh tau
quartz 1 1.e10 87.5 1.e-3
: itypkin npri nsec sig rk
 20 0 0 1. 1.2589e-18
:
: i1 i2 j1 j2 k1 k2 vol area vol area
 1 61 1 1 1 68 0.1 100.
/
calcite 1 1. 35. 1.e-3
 20 0 0 1 -10.
 1 61 1 1 1 68 0.02 1.
/
/
:
BRKP 1
1 1 52
:
DTSTep[y] 1 3.e-8
1.e-8 1.e2
:
TIME[y] 6 10. 100. 500. 1000. 5000. 10000.
:
ENDS

```


4.1.1 METRA Screen Display

When running METRA in its normal transient mode, the screen printout displays in order of appearance: step number, current time, time step size, number of Newton-Raphson iterations (with the cumulative number of iterations in parenthesis), number of time step cuts (with cumulative number of cuts in parenthesis), convergence criteria used, number of inner iterations for solver per Newtonian iterations changes in pressure, saturation, and temperature over the time step.

```

step  time [y]  dt [y]  newton  ncut  icnv <... solver (gmres) itr...>
  1  1.000E-05  1.000E-05  2(  2)  0(  0)  1  4  4
dP(  1  1  72)=  1.13E+00  dS(  1  1  72)= -4.95E-07  dT(  1  1  72)=
2.55E-03
  2  3.000E-05  2.000E-05  2(  4)  0(  0)  1  4  4
dP(  1  1  72)=  1.72E-00  dS(  1  1  72)= -9.89E-07  dT(  1  1  72)= 5.09E-03
  3  7.000E-05  4.000E-05  2(  6)  0(  0)  2  4  4
dP(  1  1  72)= 2.37E-00  dS(  1  1  72)= -1.97E-06  dT(  1  1  72)= 1.1E-02

```

By inspection of output variables `dpmx`, `dsmx`, and `dtmx` it can usually be determined which variable is limiting the time step by comparing the displayed changes with those specified in the input file in the `LIMIT` keyword. The location of grid blocks are given by indices (i, j, k). For the unstructured grid option, only the linear index is printed with j and $k = 1$.

When invoking the `STEADY` keyword, after 10 time steps an additional line appears on the screen showing how far the solution is from a steady-state based on the tolerances chosen on the `STEADY` keyword:

```

 10  1.023E-02  5.120E-03  1(  10)  0(  0)  1  1
dP(  1  1  8)= -8.54E-03  dS(  1  1  72)=  3.19E-08  dT(  1  1  72)- -
7.80E-06

 11  2.047E-02  1.024E-02  1(  11)  0(  0)  1  1
dP(  1  1  8)= -7.53E-03  dS(  1  1  72)=  6.12E-08  dT(  1  1  72)-
8.14E-06
dx/dt-->

 12  4.095E-02  2.048E-02  1(  12)  0(  0)  1  1
dP(  1  1  4)=  7.90E-03  dS(  1  1  72)=  1.16E-07  dT(  1  1  86)= -807E-06
dX/dt-->

```

When dX/dt becomes less than one for all three variables (pressure, saturation, and temperature), the solution has converged.

4.1.2 Screen Display

The GEM screen display appears as

```

      / / / / /      / / / / /      / / / / /
     / / / / /      / / / / /      / / / / /
    / / / / /      / / / / /      / / / / /
   / / / / /      / / / / /      / / / / /
  / / / / /      / / / / /      / / / / /
 / / / / /      / / / / /      / / / / /
/ / / / /      / / / / /      / / / / /

      Prepared for the U.S. NRC

              Version 1.5

              July 2001

MULTIPHASE-MULTICOMPONENT CHEMICAL TRANSPORT MODEL

      Copyright (c) 2000 Southwest Research Institute
      All Rights Reserved
  
```

Following the header information, the call to subroutine readat is indicated beginning the processing of the input file:

```
--> call readat
```

Storage requirements for the array aa are then computed based on the input data and indicated as

```

=====
Total Work Space Required for [aa] in GEM = 154100
                                         Assigned = 10000000
=====
  
```

Next, the thermodynamic database used and the numbers of primary, secondary, and mineral species are printed indicating that the database has been successfully read:

```

--> master species for time step control: h+
--> call database
--> using database: mstemp.r16
--> matrix dimension: 27
--> finished processing database
--> primary species: 10
--> secondary species: 25
--> minerals: active: 2 total: 3
  
```

After the database is read in, distribution of species calculations are performed for the initial and boundary conditions. Successful completion for each block and region and the number of iterations required are printed:

```

--> call startup
--> processing initial conditions: 2 region(s)
--> node = 1 region: 1 temp = 298.1 iter = 35
--> node = 2 region: 1 temp = 298.1 iter = 2
--> node = 3 region: 1 temp = 298.1 iter = 4
...
--> compute boundary condition at face: 3 iter = 36
--> compute boundary condition at face: 4 iter = 21

```

The code now begins time stepping. A brief message indicates the options chosen in the masin input file:

```

*****
*   Begin Mass Transport Calculation   *
*                                     *
* --> single continuum model          *
*                                     *
* --> method: Fully Implicit          *
*                                     *
* --> Finite difference algorithm: up-wind *
* --> solver: watsolv                 *
*                                     *
* --> nonisothermal system           *
*                                     *
*****

```

At each time step the GEM screen display gives the number of steps (mcytc), iterations (iter), time step cuts (ihalve), convergence criteria (iconv), solution method (ifor), time, time step, maximum time step as specified on the DTSTep keyword and the species controlling the time step (maspec). A second line displays the maximum change in concentration in solution (dc) and the maximum time rate of change (dcdt) for the indicated node and species. A third line gives the maximum change in mineral concentration (dm) for the specified node and mineral. An example is shown:

```

mcytc iter ihalve iconv ifor time   delt   dtmax [y] maspec
  1  2  0  2  2  1.000  1.000  100.0  sio2  1
--> watsolv: 1 1
--> dc = -6.7763E-20 dcdt = -6.7763E-20 at node 40 sio2(aq)
--> dm = 0. at node = 1 quartz
.....
mcytc iter ihalve iconv ifor time   delt   dtmax [y] maspec
 10  2  0  2  2  16.31  3.765  100.0  sio2  1 --> watsolv: 1 1
--> dc = 2.4395E-19 dcdt = 6.4794E-20 at node 31 sio2(aq)
--> dm = 1.9493E-18 at node = 6 quartz
.....

```



```

--> call startup
--> processing initial conditions: 2 region(s)
--> node: 1 region: 1 temp = 288.3 iter = 41
--> node: 2 region: 1 temp = 288.5 iter = 24
--> node: 3 region: 1 temp = 288.8 iter = 24
...
--> compute boundary condition at face: 3 iter = 36
--> compute boundary condition at face: 4 iter = 21

```

The code now begins time stepping. A brief message indicates the options chosen in the masin input file:

```

*****
*   Begin Mass Transport Calculation   *
*                                     *
* --> method: fully implicit          *
*                                     *
* --> routine: hybrid                 *
* --> solver: watsolv                 *
*                                     *
* --> nonisothermal system            *
*                                     *
*****

```

In coupled mode the screen display shows results at each time step from METRA and GEM successively:

```

-----[ METRA ]-----
step time [y] dt [y] newton ncut < solver (tridi) itr...>
  1 1.000E-06 1.00E-06 1( 1) 0( 0) 1
dP( 1 1 75)= 1.01E-03 dS( 1 1 77)= 6.80E-12 dT( 1 1 71)= 3.86E-09
-----[ GEM ]-----
--> boundary condition: type 3 temp = 15.0 iter = 7
--> boundary condition: type 3 temp = 30.0 iter = 7
mcyk kcyk iter iconv ifor time target delt [y] maspec ndts itrtrt
  1 1 1 2 1.0000E-08 1.0000E-08 1.0000E-08 ca+2 1 1
--> watsolv: (cgstab): 1
--> dc( 1 1114) = -1.375D-09 dcdt = -1.375D-03 ca+2 Res(5 115) 5.39D-17
--> ds( 1 1121) = 4.716E-12 sio2(am)
--> max cum err = 0.000E+00 ca+2
.....
Peclet Nr. [l,g] vl vg [m/y] cfl cfg mcyk
0.7896 1.9771E-02 2.3631E-04 7.0115E-03 8.5842E-03 8.9150E-07 1
-----[ METRA ]-----
step time [y] dt [y] newton ncut iconv < solver (tridi) trs >
  2 3.000E-06 2.00E-06 1( 2) 0( 0) 1 1
dP(1 1 79)= 1.91E-03 dS( 1 1 77)= 1.36E-11 dT( 1 1 71)= 7.77E-09
-----[ GEM ]-----
Peclet Nr. [l,g] vl vg [m/y] cfl cfg mcyk
0.7896 1.9771E-02 2.3631E-04 7.0114E-03 8.5842E-09 89046E-07 3
.....[ METRA ].....
step time [y] dt [y] newton ncut iconv < solver (tridi) trs >
  3 7.000E-06 4.00E-06 1( 3) 0( 0) 1 1
dP(1 1 79)= 3.43E-03 dS( 1 1 77)= 2.72E-11 dT( 1 1 71)= 1.55E-08

```

```

.....[ GEM ].....
Peclet Nr.   [l,g]       vl       vg [m/y]       cfl       cfg       mcyc
0.7896      1.9771E-02   2.3631E-04  7.0114E-03   4.2921E-09 4.4426E-07  6
.....[ METRA ].....
step  time [y]  dt [y]  newton  ncut  iconv < solver (tridi) trs >
  4    1.500E-05 8.000E-06 1( 4)   0( 0) 1    1
dP(1    1 79)= 5.59E-03 dS( 1 1 77)= 5.45E-11 dT( 1 1 71)= 3.09E-08
.....[ GEM ].....
mcyc kcyc iter icnv icut ifor time      target  delt [y] maspec ndts itrtdt
10   4    1    2    0    2    1.5000D-05 1.5000D-05 3.125D-06 ca+2 1    10
--> watsolv (cgstab):
--> dc( 1 114)= 4.298D-09 dcdt = -1.375D-03 ca+2 Res(5 116) 5.26D-16
--> ds( 1 1121) = 1.474E-11 sio2(am)
--> max cum err = 9.204E-10 sio2(aq)
.....
Peclet Nr.   [l,g]       vl       vg [m/y]       cfl       cfg       mcyc
0.7896      1.9771E-02   2.3631E-04  7.0113E-03   2.6826E-03 2.7659E-06 10
.....[ METRA ].....
step  time [y]  dt [y]  newton  ncut  iconv < solver (tridi) trs >
  5    3.100E-05 1.600E-05 1( 5)   0( 0) 1    1
dP(1    1 79)= 7.78E-03 dS( 1 1 77)= 1.09E-10 dT( 1 1 77)= 6.31E-08
.....[ GEM ].....

```

The screen output described for METRA remains the same in the MULTIFLO output with the header repeated at each step. The GEM display is slightly modified to show the inner number of GEM steps within a single METRA time step (*kcyc*). The maximum time step is not displayed in this case. The beginning with --> watsolv indicates the number of WATSOLV iterations for each outer iteration indicated by *iter*.

4.2 METRA Output

The items are discussed in the order in which they appear in a typical output file and grouped as Initialization and Recurrent Output sections.

4.2.1 Initialization Output

4.2.1.1 Mass and Energy in Place

These values are computed by simply summing the mass and energy content of each grid block:

$$\text{Mass}_i = PV (D_w S_w + D_g S_g) X_i MW_i, \quad (4-1)$$

for *i*th component,

$$\text{Energy} = PV(D_w S_w U_w + D_g S_g U_g) + VB(1-Por) D_r C_p T, \quad (4-2)$$

where

PV	—	Pore volume of a grid block [m^3]
D_w	—	Liquid molar density [moles/ m^3]
D_g	—	Gas molar density [moles/ m^3]
S_w	—	Liquid saturation [fraction]
S_g	—	Gas Saturation [fraction]
X_i	—	Mole fraction of the i th component
MW_i	—	Molecular weight of the i th component
VB	—	Bulk block volume [m^3]
Por	—	Porosity [fraction]
D_r	—	Rock density [Kg/m^3]
Cp_r	—	Rock specific heat [$J/kg-C$]
T	—	Temperature [$^{\circ}C$]
U_w	—	Molar internal energy of liquid [$J/mole$]
U_g	—	Molar internal energy of gas [$J/mole$]

Bulk volume of a block for Cartesian and the cylindrical geometries are computed as

$$V_B = DX * DY * DZ, \quad (4-3)$$

for Cartesian geometry,

$$= \pi (r_{i+1/2} + r_{i-1/2}) (r_{i+1/2} - r_{i-1/2}) DZ, \quad (4-4)$$

for cylindrical geometry, where

DX, DY, DZ	—	Block dimensions in x-, y-, and z-direction
π	—	3.14159
$r_{i+1/2}$	—	Outer radius of i th block
$r_{i-1/2}$	—	Inner radius of i th block

The pore volume of a block (PV) is computed as $VB - Por$.

4.2.1.2 Initial Conditions

Initial condition variables include pressure (P), temperature (T), gas saturation (S_g), and mole fraction of air component (X_g^a). In a two-phase region, X_g^a is a function of P and T , computed using the ideal gas law as

$$X_g^a = (P - P_v) / P, \quad (4-5)$$

where

$$P_v = \text{saturation pressure of water.} \quad (4-6)$$

Vapor pressure P_v is only a function of T if the effect of capillary pressure on vapor pressure is neglected. If the effect of capillary forces, on vapor pressure is taken into account P_v is a function of capillary pressure, liquid water density, temperature, and saturation pressure.

4.2.1.3 Transmissibility

The constant coefficients of fluid transmissibility (T_x , T_y , and T_z) are interblock properties and calculated in each direction as follows—for Cartesian Geometry

$$T_{x_i} = \frac{2\kappa_i \kappa_{i-1} \Delta y \Delta z_k}{\Delta x_i \kappa_{i-1} + \Delta x_{i-1} \kappa_i} \quad (4-7)$$

$$T_{y_i} = \frac{2\kappa_j \kappa_{j-1} \Delta x_i \Delta z_k}{\Delta y_j \kappa_{j-1} + \Delta y_{j-1} \kappa_j} \quad (4-8)$$

$$T_{z_k} = \frac{2\kappa_k \kappa_{k-1} \Delta x \Delta y_j}{\Delta z_k \kappa_{k-1} + \Delta z_{k-1} \kappa_k} \quad (4-9)$$

where κ_i and κ_{i-1} are the permeability values in i -direction (x or r) for i th and $(i-1)$ st blocks. Similarly, κ_j , κ_{j-1} , and κ_k , κ_{k-1} are values in y or angular and vertical directions. For Cylindrical Geometry:

$$T_{x_i} = \frac{2\pi \kappa_i \kappa_{i-1} \Delta y \Delta z_k}{\kappa_{i-1} \ln \frac{r_i}{r_{i-1/2}} + \kappa_i \ln \frac{r_{i-1/2}}{r_{i-1}}} \quad (4-10)$$

$$T_{z_k} = \frac{2\kappa_k \kappa_{k-1} \Delta x \Delta y_j}{\Delta z_k \kappa_{k-1} + \Delta z_{k-1} \kappa_k} \quad (4-11)$$

The block center radius for a cylindrical system is r_i where $r_{i-1/2}$ and $r_{i+1/2}$ are the inner and outer radii of the block boundaries.

For a cylindrical system, the transmissibilities are multiplied by a factor ($\text{angle}/2\pi$) if the system is not a full 360° .

Since the transmissibilities are at block interfaces, they correspond to the space location at $(i_{j-1/2}, j, k)$ between blocks i and $i-1$, and similarly in j and k directions. The transmissibility between i th and $(i-1)$ st block is designated as the i th transmissibility.

For an unstructured grid the transmissibility has the form for the connection between nodes m_1 and m_2 .

$$T_{m_1, m_2} = \frac{2\kappa_{m_1}\kappa_{m_2}A_{m_1, m_2}}{d_{m_2}\kappa_{m_1} + d_{m_1}\kappa_{m_2}}, \quad (4-12)$$

4.2.1.4 Binary-Diffusion Transmissibility

In the presence of vapor-air binary diffusion, the constant coefficients corresponding to these transmissibilities (T_{x_i}, T_y, T_z) are calculated from Eq. (4-13)

$$T_{x_i} = \frac{\omega\sqrt{\phi_i\tau_i\phi_{i-1}\tau_{i-1}}D_{va}^0\Delta y_j\Delta z_k}{RT_0^\theta(\Delta x_i + \Delta x_{i-1})} \quad (4-13)$$

and similarly in y - and z -directions, where

- ω — enhancement factor
- τ — tortuosity factor
- ϕ — porosity
- D_{va}^0 — binary diffusion coefficient [m^2/s] (read in as CDIFF with THERM keyword)
- θ — exponent in the relation (read in as CEXP)
- T_0 — 273.15 (absolute temperature at 0 °C)

4.2.2 Recurrent Output

4.2.2.1 Mass and Energy in Place

Mass and energy in place at any time (t) and are computed in a manner identical to the initial values

4.2.2.2 Inner Iteration Counter

The output variable INRITRS represents the number of inner iterations during each Newtonian iteration and their sum over a time step. The inner iterations correspond to the number of iterations required for convergence by an iterative solver. For direct solvers such as band-solve, the number of Newtonian iterations is equal to the number of inner iterations and, therefore, they are not printed when the direct method is specified as the solver. Note that one-dimensional systems are solved by the direct method as default. The number of

Newtonian iterations required for convergence corresponds to the number of times a linearized equation solver is called, excluding the call to the solver when a time step cut was performed.

4.2.2.3 Err-H₂O, Err-Air, Err-Enrg

The output variables **Err-H₂O**, **Err-Air**, and **Err-Enrg** represent an estimate of the errors in the solution over a time step. Thus, these numbers identify the mass (kg) or energy (joules) of H₂O, air, and energy unaccounted for in the solution at the end of a time step. **Err-H₂O** is computed as follows:

$$\text{Err-H}_2\text{O} = M_{\text{H}_2\text{O}}(t + \Delta t) - M_{\text{H}_2\text{O}}(t) - M_{\text{H}_2\text{O}} \text{ mass injected} \quad (4-14)$$

Err-Air and **Err-Enrg** for air and energy are calculated analogously.

The solution errors can be reduced by tighter tolerances (TOLR-Keyword) at the expense of increased computing time. Because of machine round-off errors (number of significant digits for computations), these errors cannot be reduced beyond certain finite values. In practical terms, a small solution error implies the results are reasonably accurate.

4.2.2.4 ICONV

The variable **ICONV** assumes a value of 1 or 2 and indicates if convergence is achieved based on maximum changes in the solution variables (**ICONV=1**) or in the residual errors (**ICONV=2**).

Thus, for **ICONV = 1**,

$$\max_n | \Delta p_n^k, \Delta p_{an}^k, \Delta s_n^k, \Delta T_n^k | < [tolp, tolpa, tols, tolt], \quad (4-15)$$

where κ is the Newtonian iteration number, n refers to the node, and Δp_n^k , Δp_{an}^k , Δs_n^k , and ΔT_n^k represent the solution vectors. The parameters *tolp*, *tolpa*, *tols*, and *tol* corresponding to total pressure, partial pressure of air, saturation, and temperature are specified as the first four variables in the TOLR keyword.

The next three variables on the TOLR keyword control the convergence for **ICONV = 2**. For **ICONV = 2**,

$$\max_n | R_{in}^k | < [tolm, tola, tole] \quad (4-16)$$

where R_{in}^k represents the normalized residual at the n th node and k th iteration for the i th conservation equation ($i = 1, 2$, and 3 corresponding to total mass, air and energy) and *tolm*, *tol*, and *tole* are the specified tolerances. If convergence is desired based on only **ICONV = 1** or **2**, the parameters corresponding to the undesired criteria may be set to a small number

(e.g., 1.e-30). The residual is normalized by dividing the residual error by the block mass and energy in place at the current time.

4.2.2.5 DPMAX, DSMAX, and DTMPMX

These variables denote the maximum change in pressure, gas saturation, and temperature over a time step. The block that undergoes such a maximum change is identified in parentheses with reference to its (i, j, k) location.

4.2.2.6 Balances

Similar to $Err-H_2O$, etc., the balance is another indicator of the accuracy of the solution. Two different types of balances are computed: cumulative and incremental. The cumulative balance becomes relatively less sensitive after a sufficient amount of fluid/energy is injected/produced (including influx and efflux) but reflects the overall error in the system from the initial time. Thus, a significant error during a few time steps may not reflect adversely on the cumulative balance. The incremental balance takes cognizance of the error only over a time step. Balances for H_2O , air, and energy are printed as H_2OBAL , $AIRBAL$, and $ENRGBAL$. H_2OINC , $AIRINC$, and $ENGINC$ represent the corresponding incremental balances.

For a perfect solution, both the incremental and cumulative balances should be unity. Note that if there is zero net injection/influx, the balance calculations result in an indeterminate quantity. In this case, monitoring the errors, $Err-H_2O$, etc., provides the needed control to assess the accuracy of the solution.

Balances are saved in a separate file, `lfn_bal`, that should be reviewed at the end of each run to ensure satisfactory results.

4.2.2.7 Boundary Condition Influx Summary

The variables designated as `cummbc`, `cumcbc`, and `cumhbc` represent the cumulative mass, air mass, and total energy influx from time = 0 into the system. Negative values represent flux out of the system. The rate of influx for the corresponding quantities is given by q_m , q_a , and q_h .

4.2.2.8 Source/Sink Summary

The printout is analogous to the boundary condition influx with similar meaning of the variables.

4.2.2.9 Velocities

The velocities represent superficial Darcy velocities. They are computed at block interfaces in `lfn_out` file and at the block center in the plot files. For the dual continuum model, fracture-matrix interfacial velocities are defined as positive for flow from fracture to matrix.

4.2.2.10 Plot Files

A number of plot files are written in spreadsheet format for ease in plotting results. Both spatial profiles printed at target times and time-history plots at specified node points are available. Time-history plots consist of five files with the variables shown in Table 4-1.

For a system represented by a single continuum, there are two spatial plot files: one for field variables and one for flow velocities and fluxes. For the dual continuum model option, separate files for matrix and fracture fields are written. The units for velocity are meters per input time unit. Fluxes are in units of kg/m²/s. The structure of the spatial plot files is shown in Table 4-2.

4.2.2.11 Other Files

The disk files listed in Table 4-3 are automatically opened on initiation of a run. The names of the files are assigned based on the name of the input data file as indicated in the table with the prefix *fn*.

The files are closed on successful completion of a run. The data file must have the extension *.dat*. The output files have a suffix separated by *_* (underscore).

To restart a run from a saved restart file *fn_rso*, change the name of the restart file to *fn_rsi*.

4.3 GEM Output

The default output file for GEM is called *masout*. This file echos back the input data, lists the thermodynamic data for each reaction, and provides results of the distribution of species calculations for the initial and boundary fluid compositions. A number of plot files are written depending on the specifications in the *PLTFiles* keyword. All plot files are in ASCII with a spread sheet format and can be read and edited by almost any text editor. Comment lines beginning with an exclamation mark (!) appear at the top of each file labeling the various columns and providing the target time corresponding to the file. The *n* in square brackets (*[n]*) labels the plot file with the *n*th target time. Plot file names are listed in Tables 4-4 and 4-5.

Table 4-1. List of Time-History Plot Files and Associated Variables	
File Name	Variable
jobname_his.xyp	time step
jobname_tmp.xyp	temperature
jobname_sat.xyp	saturation
jobname_press.xyp	pressure
jobname_rh.xyp	relative humidity

Table 4-2. List of METRA Plot Files Printed at Target Times and Associated Variables for Plotting Spatial Data	
File Name	Variables
jobname_fld.xyp	[xyz], press, temp, sl, sg, xairl, xairg, pcap
jobname_flx.xyp	[xyz], vgx, vlx, vgy, vly, vgz, vlz, fgx, fix, fgy, fly, fgz, flz

Table 4-3. Unit Numbers and Associated Files		
Unit	File Name	Description
51	fn.dat	Input data file
52	fn.out	Output file
53	fn_errs	Run errors and diagnostics file
53	fn_bal	Energy and mass balance file
55	fn_vel	Velocity file
56	fn_rsi	Restart file to resume a run
57	fn_rso	Restart file
58	fn_bug	Debut output file
59	fn_prn	Monitoring file
60	fn.bc	Boundary condition data
60	fn.int	Initial condition data
60	fn.pck	Material properties data
60	fn.phk	Porosity/permeability data
60	fn.src	Source data

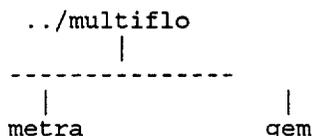
Table 4-4. List of Plot Files Containing Spatial Profile Data at Times Specified on the TIME Keyword	
File Name	Description
maspltaq[n].xyp	Aqueous concentrations
maspltele [n].xyp	Electrochemical potential
maspltgas [n].xyp	Gaseous species concentrations
maspltmin [n].xyp	Mineral reaction rates
maspltpsi [n].xyp	Total aqueous concentrations
maspltsat [n].xyp	Mineral saturations
maspltsec [n].xyp	Aqueous secondary species concentrations
maspltsor [n].xyp	Sorbed species concentrations
maspltsrf [n].xyp	Mineral surface area
maspltvol [n].xyp	Mineral volume fractions
table.tex	LaTeX or ASCII formatted table containing the inlet solution composition

Table 4-5. List of Plot Files Containing Time-history Data at Spatial Nodes Specified on the BRKP Keyword	
File Name	Description
maspltbrk.xyp	Break-through concentrations
maspltini.xyp	Inlet concentrations
maspltznb.xyp	Positions of reaction zone boundaries

5 INSTALLATION AND EXECUTION

5.1 Installation

The following instructions apply to a UNIX operating system. The source code for MULTIFLO is installed in a hierarchical directory structure. The topmost level directory (e.g., ../multiflo) contains the main program for MULTIFLO and the source code for sequentially coupling METRA and GEM. In addition, there are two subdirectories containing the source code for METRA and GEM.



The default thermodynamic databases for GEM, master25.V8.R5 and mastertemp.V8.R5, are stored in the directory database located in the user's home directory under the ~/bin subdirectory (the subdirectory ~/bin must be in the user's search path in the .cshrc file): ~/bin/database.

The include files, paramtrs.h, impl.h, metragem.h, and watsolv.h, must be identical in the METRA and GEM subdirectories.

To compile the code, type

```
make multiflo
```

in the top level directory to create the MULTIFLO executable. Type

```
make metra
```

in the METRA subdirectory to create the stand alone METRA executable. Type

```
make gem
```

in the GEM subdirectory to create the stand alone GEM executable.

For the executables to be accessible in any subdirectory in the user's home directory, make soft links to the subdirectory ~/bin as follows:

```
mkdir ~/bin      (if directory does not exist)
cd ~/bin
ln -s ../multiflo/multiflo
ln -s ../multiflo/metra/metra
ln -s ../multiflo/gem/gem
```

These commands assume the directory `multiflo` is located in the user's home directory. The subdirectory `~/bin` must appear in the user's search path in the `.cshrc` file.

5.2 Execution of MULTIFLO, GEM, and METRA

5.2.1 MULTIFLO

To run MULTIFLO, type

```
multiflo
```

A prompt will appear

```
-->enter icode: (1-metra, 2-gem, 3-coupled, 4-coupled: steady-state)
```

After the prompt, the user enters a single digit in the range 1-4 to select the mode of operation desired.

Input files for GEM and METRA with the names `masin` and `multi.dat` must be present in the current directory. Additional input files may also be required for (e.g., initial conditions depending on the run options).

5.2.2 GEM

It is possible to run the stand-alone version of GEM by typing

```
gem [options]
```

The command-line options allow the default assignment of files names to be overridden. The options available may be displayed by entering the command: `gem -x`

```
[-i]      <masin>
-o        <masout>
-a        <maspltaq>
-s        <maspltsec>
-t        <maspltpsi>
-d        <data1>
-m        <maspltmin>
-si       <maspltsat>
-sf       <maspltsrf>
-v        <maspltvol>
-z        <maspltznb>
-b        <maspltbrk>
-l        <maspltini>
-ex       <maspltsor>
-g        <maspltgas>
-r        <restart>
```

The names in brackets <...> denote default file names. These options are available only in stand-alone mode.

5.2.3 METRA

The stand-alone version of METRA is run by typing

```
metra file
```

where `metra` is the name of the executable module and `file.dat` is the name of the input data file. The data file name should not be longer than seven characters and MUST have `.dat` as the extension. This command will execute the job interactively.

If the job is to be processed in background mode, type

```
metra file &
```

or

```
nohup metra file &
```

Note the output files will have names with the same prefix as the data file prefix. This enables simultaneous execution of different data sets having different names in the same subdirectory.

On completion of a run or abnormal termination, carefully examine the `fn_bal` (balance) and the `fn_errs` (error) files, where `fn` refers to the input data file, to ensure there are no errors and mass and energy balances are reasonably conserved. For a near perfect solution, the cumulative balances should not deviate from unity more than 0.1 percent. The incremental balances may vary more sporadically.

5.3 Redimensioning

Occasionally, the user may need to modify the array sizes to increase the number of grid blocks, number of primary species, aqueous complexes, minerals, gases, or other properties of the system. In addition, it may be necessary to modify the main storage array `aa` in the main program. The value of `maxaa` must be changed to the same value as the dimension for the array `aa`. This is done in `maingem.` and `mainmetra.` for stand alone mode and `mainmlti.f` in the top level directory for running the code in coupled mode.

For different-sized problems, it may be desirable or even necessary to alter the dimensions of certain arrays. There are two places in the code where the array sizes can be altered.

- Modify the dimensioning parameters in file `paramtrs.h` listed below. Note for the dual continuum model option, `nmbx = 2*nx*ny*nz`, (i.e., `nmbx`) must be twice the actual number of grid blocks used in the calculation.

```

c*comdeck paramtrs.h

c reqd for both gem and metra.
c See below for definition of variables.

parameter (Nxxmx = 600, nymx = 200, nxmz = 750, nbmx = 2000,
           Nconmx = 4000, nbcmx = 10, nblkbcmx = 200)

c for minc formulations
parameter (mnc = 5\7, mncp = mnc+1, mnmx = 1000) !mnmx .LE. nbmx

c reqd for metra only

parameter (nxmx = 100,
           nstbmx = 100,
           nrkmx = 100,
           ntbcmx = 100)

c reqd for gem only

parameter (nsmx = 16,
*          ncxmx = 70,
*          nxkmx = 6,
*          nmmx = 50,
*          nkmx = 50,
*          ngmx = 6,
*          nxemx = 4,
*          ntmpmx = 10,
*          ndimmx = nmmx+ncxmx+ngmx+nxkmx,
*          nscmx = 2,
*          nscxmx = 10,
*          nrgmx = 20, ! sum of comp. regns + BC + source/sink
*          nsrcms = 5) ! max no. of source/sink

parameters (ncxmx0 = 300, nmmx0 = 300, ngmx0 = 10)

c definition of parameters
c   nxmx      = max no. of elements in i-direction
c   nymx      = max no. of elements in j-direction
c   nzmx      = max no. of elements in k-direction
c   nbmx      = max no. of total elements
c   nbcmx     = max no. of boundary condition regions
c   nblkbcmx  = max no. of BC blocks in all regions

c definition for min formulation
c   mnc       = no. if interacting continua within a block excluding
               fracture
c   mncp      = no. of continua within a block including the fracture
               continuum.
c   mnmx      = no. of minc blocks < or = nbmx.

c =====following for metra only=====

c   nsmx      = max no. of total source/sink
c   nstbmx    = max no. of time entries in source/sink tables

```

```

c      nrkmx      = max no. of rock-types (different pc and kr functions)
c      ntbcmx     = max no. of time entries in boundary condition tables
c
c =====following for gem only=====
c
c      ncmx       = maximum number of primary species
c      ncxmx      = maximum number of aqueous complexes
c      nxkmx      = maximum number of irreversible aqueous reaction
c      nmmx       = maximum number of minerals
c      nkmx       = maximum number of kinetically reacting minerals (nk<=nm)
c      ngmx       = maximum number of gases
c      nzemx      = maximum number of reaction zones in printout
c      ntmpmx     = maximum number of temperatures in database
c      nrgmx      = maximum number of regions specified in COMP and BCON
c      nscmx      = maximum number of source/sink
c      nscxmx     = maximum number of sorption reactions (surface complexes)
c ends

```

- If during execution the run terminates because of insufficient size of array `aa` in the main program, reset the array size to a larger value. Also, the data statement `maxaa` must be reset to the same value as the dimensions of the `aa` array. Prior to the termination of a run, a message will be printed indicating the minimum required size of array `aa`.

5.4 Machine Specific Routines

Since different computing systems use different system timing routines, a call to the appropriate timing routine for a particular system should be invoked. This should require a change only in the `seconds.f` subroutine within the `cputim.f` group of routines. At present, it is set for SUN workstations. Calls to timing routines for the Lahey compiler for PC and LPI compiler for PC/UNIX are deactivated. The timing routine should compute the time in CPU-seconds. Beside `dtime()` and `etime()`, other machine specific routines are `rand()` for computing random numbers and `date()` providing a date and time stamp in the output files for GEM and METRA.

5.5 Compilation

Makefiles are included with the source code. The code is written in double precision, so no special compiler options for double precision should be specified. For Cray and other 64-bit machines, the statement `implicit real*8 (a-h,o-z)` in `impl.h` file should be commented out. The executable files MULTIFLO, GEM, and METRA are produced.

6 REFERENCES

Appelo, C.A.J. "Multicomponent Ion Exchange and Chromatography." *Reactive Transport in Porous Media*. P.C. Lichtner, C.I. Steefel, and E.H. Oelkers, eds. *Reviews in Mineralogy*. Vol. 34. pp. 193–227. 1996.

Goossens, M., F. Mittelbach, and A. Samarin. *The Latex Companion*. New York City, New York: Addison Wesley Publishing Company. 1994.

Hirschfelder, J.O., C.F. Curtiss, and R.B. Bird. *Molecular Theory of Gases and Liquids*. New York, New York: John Wiley & Sons. 1954.

International Formulation Committee. "A Formulation of the Thermodynamic Properties of Ordinary Water Substance." Dusseldorf, Germany: IFC Secretariat. 1967.

Lichtner, P.C. "Continuum Formulation of Reactive Transport." *Reactive Transport in Porous Media*. P.C. Lichtner, C.I. Steefel, and E.H. Oelkers, eds. *Reviews in Mineralogy*. Vol. 34. pp. 1–81. 1996.

Lichtner, P.C. and J.C. Walton. "Near-Field Liquid-Vapor Transport in a Partially Saturated High-Level Nuclear Waste Repository." CNWRA 94-022. San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. 1994.

Nitao, J.J. "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. Livermore, California: Lawrence Livermore National Laboratory. 1989.

van der Kwaak, J.E., P.A. Forsyth, K.T.B. MacQuanie, and E.A. Sudicky. "WATSOLV, Sparse Matrix Iterative Solver Package, User's Guide." Waterloo, Ontario, Canada: Waterloo Centre for Groundwater Research, University of Waterloo. 1995.

Warren, J.E., and P.J. Root. "The Behavior of Naturally Fractured Reservoirs." *Society Petroleum and Engineers Journal*. Vol. 3. pp. 245–255. 1963.

Wolery, J.J. "EQ3NR, A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations: Theoretical Manuals, User's Guide, and Related Documentation. Version 7.0. UCRL-MA-110662 PT III. Livermore, California: Lawrence Livermore National Laboratory. 1992.

APPENDIXES

METRA

This appendix provides a brief mathematical description of the underlying equations solved by METRA.

A.1 SATURATION FUNCTIONS

Capillary saturation functions provided in METRA are van Genuchten (1980), linear, and Brook-Corey functions. In addition, tabular data may be provided by the user.

A.1.1 van Genuchten Saturation Functions

Capillary pressure is related to saturation by various phenomenological relations, one of which is the van Genuchten (1980) relation given by

$$s_l^{\text{eff}} = [1 + (\alpha |P_c|)^m]^{-\lambda}, \quad (\text{A-1})$$

where P_c represents the capillary pressure [Pa], and s_l^{eff} is defined by

$$s_l^{\text{eff}} = \frac{s_l - s_l^r}{s_l^0 - s_l^r}, \quad (\text{A-2})$$

where s_l^r denotes the residual saturation, and s_l^0 denotes the maximum saturation. The quantity m is related to λ by the expression

$$\lambda = 1 - \frac{1}{m}, \quad m = \frac{1}{1 - \lambda}. \quad (\text{A-3})$$

Relative permeability for the liquid phase is given by the expression and for the gas phase by

$$k_{rl} = \sqrt{s_l^{\text{eff}}} \left\{ 1 - \left[1 - (s_l^{\text{eff}})^{1/\lambda} \right]^\lambda \right\}^2, \quad (\text{A-4})$$

and for the gas phase by

$$k_{rg} = 1 - k_{rl}. \quad (\text{A-5})$$

A.1.2 Brook-Corey Functions

The Brook-Corey functions for relative permeability are defined by

$$k_{rl} = s_*^4, k_{rg} = (1 - s_*^2)(1 - s_*)^2, s_* = \frac{s_l - s_l^r}{1 - s_l^r - s_g^r}. \quad (\text{A-6})$$

Capillary pressure is not incorporated in the Brook-Corey functions.

A.1.3 Linear

The linear relation is defined by

$$k_{rl} = s_*, k_{rg} = 1 - k_{rl}, s_* = \frac{s_l - s_l^r}{1 - s_l^r}. \quad (\text{A-7})$$

A.2 KELVIN'S EQUATIONS FOR VAPOR PRESSURE LOWERING

Vapor pressure lowering resulting from capillary suction is described by Kelvin's equation given by

$$P_v = P_{\text{sat}}(T) e^{-P_c n_l / RT}, \quad (\text{A-8})$$

where P_v represents the vapor pressure, P_{sat} the saturation pressure of pure water, T denotes the absolute temperature and R denotes the gas constant. Note that the density of the liquid phase, n_l , is represented on a molar basis.

A.3 THERMAL CONDUCTIVITY

Thermal conductivity is determined from the equation (Somerton, et al., 1974)

$$CK = CK_{\text{DRY}} + \sqrt{s_l} (CK_{\text{SAT}} - CK_{\text{DRY}}), \quad (\text{A-9})$$

where CK_{DRY} and CK_{SAT} are dry and fully saturated rock thermal conductivities.

A.4 VAPOR-AIR DIFFUSION EQUATION

The conservation equation for the H₂O component (*w*) is given by

$$\begin{aligned} & \frac{\partial}{\partial t} [\phi (s_l n_l X_w^l + s_g n_g X_w^g)] \\ & + \nabla \cdot (q_l n_l X_w^l + q_g n_g X_w^g - D_g^{\text{eff}} n_g \nabla X_w^g) = Q_w, \end{aligned} \quad (\text{A-10})$$

and for the air component (*a*) by

$$\begin{aligned} & \frac{\partial}{\partial t} [\phi (s_l n_l X_a^l + s_g n_g X_a^g)] \\ & + \nabla \cdot (q_l n_l X_a^l + q_g n_g X_a^g - D_g^{\text{eff}} n_g \nabla X_a^g) = Q_a, \end{aligned} \quad (\text{A-11})$$

with source terms Q_w and Q_a . In these equations, the Darcy fluxes for liquid, q_l , gas, and q_g , are defined by

$$q_l = - \frac{\kappa \kappa_l}{\mu_l} \nabla (P_l - \rho_l g z), \quad (\text{A-12})$$

and

$$q_g = - \frac{\kappa \kappa_g}{\mu_g} \nabla (P_g - \rho_g g z), \quad (\text{A-13})$$

where κ denotes the saturated permeability, $P_{l,g}$ the fluid pressure, $\mu_{l,g}$ the viscosity of the liquid and gas phases with mass densities $\rho_{l,g}$ and g the acceleration due to gravity. The quantities $n_{l,g}$ refer to the density of the liquid and gas phases based on a molar representation. The mole fractions $X_w^{l,g}$ and $X_a^{l,g}$ satisfy the relations

$$X_w^l + X_a^l = 1, \quad X_w^g + X_a^g = 1. \quad (\text{A-14})$$

Diffusion of water in the aqueous phase is neglected. The liquid and gas pressures are related through the capillary pressure:

$$P_l = P_g - P_c, \quad (\text{A-15})$$

The effective binary gas diffusion coefficient is defined in terms of temperature, pressure, and material properties by

$$D_g^{\text{eff}} = \omega \tau \phi S_g D_g^0 \frac{P_0}{P} \left[\frac{T + T_0}{T_0} \right]^\theta, \quad (\text{A-16})$$

where T_0 and P_0 denote reference temperature and pressure, θ is an empirical constant, and ω is an enhancement factor (Walton and Lichtner, 1995). The enhancement factor is usually considered to be inversely proportional to the gas saturation, S_g , which thus cancels from the expression for the effective gas diffusion coefficient.

Adding Eqs. (A-10) and (A-11) eliminates the diffusive terms providing the total mass balance equation for air and water as:

$$\frac{\partial}{\partial t} [\phi (s_l n_l + s_g n_g)] + \nabla \cdot (q_l n_l + q_g n_g) = Q_w + Q_a. \quad (\text{A-17})$$

A.5 ENERGY BALANCE EQUATION

The energy balance equation, assuming thermodynamic equilibrium between rock and fluid, is given by

$$\begin{aligned} \frac{\partial}{\partial t} [\phi (s_l n_l U_l + s_g n_g U_g)] + \nabla \cdot (q_l n_l H_l + q_g n_g H_g) \\ + \frac{\partial}{\partial t} [(1 - \phi) C_p^{\text{rock}} \rho_{\text{rock}} T] - \nabla \cdot \kappa \nabla T + Q_s. \end{aligned} \quad (\text{A-18})$$

where T denotes the temperature, U_π the total internal energy, and H_π the total enthalpy of the π th fluid phase, C_p^{rock} the heat capacity, κ the thermal conductivity, and Q_s a source term. Heat produced by chemical reactions is ignored in the present version of the code.

Together with appropriate initial and boundary conditions, the mass conservation equations for air, Eq. (A-11), the total mass balance equation, Eq. (A-17), and the heat balance equation [Eq. (A-18)] are solved simultaneously using an implicit finite difference scheme. Upstream weighting is employed at interfaces at which a change in phase occurs.

A detailed description of the equivalent continuum model can be found in Lichtner and Walton (1994).

A.6 DUAL CONTINUUM MODEL FORMULATION

Input parameters to the dual continuum model consist of the fracture volume ϵ_f and matrix block size l_x , l_y , and l_z . From these quantities the fracture aperture 2δ and fracture-matrix interfacial area per bulk volume A_{fm} follows. Depending on whether the system is one-, two-, or three-dimensional, different expressions arise for the fracture aperture and fracture-matrix surface area. The fracture aperture is obtained from the identity

$$V_m = (1 - \epsilon_f) V(\delta) \quad (\text{A-19})$$

The interfacial surface area per bulk volume is computed from the relation

$$A_{fm} = \eta a_{fm}, \quad (\text{A-20})$$

where a_{fm} refers to the interfacial surface area of a single matrix block, and η denotes the density of matrix blocks.

One-dimensional Geometry. In a one-dimensional system the fracture aperture δ is simply

$$2\delta = l \frac{\epsilon_f}{1 - \epsilon_f}, \quad (\text{A-21})$$

and the interfacial area per bulk volume

$$A_{fm} = \frac{2(1 - \epsilon_f)}{l}, \quad (\text{A-22})$$

where $l = l_x = l_y = l_z$ represents the matrix block size.

Two-dimensional Geometry. In a two-dimensional system

$$V = (l_x + 2\delta)(l_y + 2\delta) \quad (\text{A-23})$$

and

$$V_m = l_x l_y \quad (\text{A-24})$$

It follows that δ satisfies the quadratic equation

$$\delta^2 + \frac{1}{2}(l_x + l_y)\delta - \frac{\epsilon_f l_x l_y}{4(1 - \epsilon_f)} = 0. \quad (\text{A-25})$$

Solving this equation explicitly for 2δ yields the relation

$$2\delta = \frac{1}{2} \left\{ \sqrt{(l_x + l_y)^2 + 4 \frac{\epsilon_f l_x l_y}{1 - \epsilon_f}} - (l_x + l_y) \right\}. \quad (\text{A-26})$$

Three-dimensional Geometry. In a three-dimensional system

$$V = (l_x + 2\delta)(l_y + 2\delta)(l_z + 2\delta) \quad (\text{A-27})$$

and

$$V_m = l_x l_y l_z \quad (\text{A-28})$$

The aperture satisfies the cubic equation

$$\delta^3 + b\delta^2 + c\delta + d = 0, \quad (\text{A-29})$$

where

$$b = l_x + l_y + l_z, \quad (\text{A-30})$$

$$c = l_x l_y + l_y l_z + l_z l_x, \quad (\text{A-31})$$

$$d = - \frac{\epsilon_f}{1 - \epsilon_f} l_x l_y l_z. \quad (\text{A-32})$$

This equation has the explicit solution

$$\delta = \alpha + \beta - \frac{b}{3}, \quad (\text{A-33})$$

where

$$\alpha = \left(\frac{u_2 + u_3}{2} \right)^{1/3} \quad (\text{A-34})$$

$$\beta = \left(\frac{u_2 - u_3}{2} \right)^{1/3} \quad (\text{A-35})$$

and

$$u_2 = - \left[d - \frac{1}{3} bc + \frac{2}{27} b^3 \right], \quad (\text{A-36})$$

$$u_3 = \left[u_2^2 + \frac{4}{27} \left(c - \frac{b^2}{3} \right)^3 \right]^{1/2}. \quad (\text{A-37})$$

Interfacial Surface Area. Let η represent the number of matrix blocks each of volume $l_x l_y l_z$ per unit bulk volume V :

$$\eta = \frac{V_m}{l_x l_y l_z} \quad (\text{A-38})$$

The number density η/V giving the number of matrix blocks per bulk volume is equal to

$$\frac{\eta}{V} = \frac{1 - \epsilon_f}{l_x l_y l_z} \quad (\text{A-39})$$

The interfacial area per matrix block is equal to

$$a_{fm} = 2(l_x l_y + l_y l_z + l_z l_x) \quad (\text{A-40})$$

Hence in three-dimensional the interfacial area per bulk volume is equal to

$$\begin{aligned} A_{fm}^{3D} &= \frac{\eta}{V} a_{fm}, \\ &= (1 - \epsilon_f) \frac{2(l_x l_y + l_y l_z + l_z l_x)}{l_x l_y l_z}, \\ &= 2(1 - \epsilon_f) \left[\frac{1}{l_x} + \frac{1}{l_y} + \frac{1}{l_z} \right]. \end{aligned} \quad (\text{A-41})$$

In two-dimensional:

$$A_{im}^{2D} = 2(1 - \epsilon_f) \left[\frac{1}{l_x} + \frac{1}{l_y} \right], \quad (A-42)$$

and in one-dimensional:

$$A_{im}^{1D} = 2(1 - \epsilon_f) \frac{1}{l}. \quad (A-43)$$

A.7 MULTIPLE INTERACTING CONTINUUM IMPLEMENTATION

The multiple interacting continuum model described by Pruess (1983) and Pruess and Narasimhan (1982) is not supported in this version. The multiple interacting continuum model differs from the dual continuum model in that the matrix continuum is discontinuous rather than continuous. Each matrix block is discretized as a nested set of volume elements with only the outer most element connected to the fracture continuum. Distinct matrix blocks are not connected to one another. The multiple interacting continuum model can still be implemented by using the unstructured grid option with nodal connections defined in a manner consistent with nested matrix elements. However, the computational efficiency of this implementation of multiple interacting continuum will be poor compared to the decomposition procedure described in Seth and Hanano (1995).

A.8 REFERENCES

Lichtner, P.C. and J.C. Walton. "Near-field Liquid-Vapor Transport in a Partially Saturated High-Level Nuclear Waste Repository." CNWRA 94-022. San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. 1994.

Pruess, K. "GMINC-A Mesh Generator for Flow Simulations in Fractured Reservoirs. LBL-15227. Berkeley, California: Lawrence Berkeley Laboratory. 1983.

Pruess, K. and T.N. Narasimhan. "A Practical Method for Modeling Fluid and Heat Flow in Fractured Porous Media." Paper SPE-10509. *Proceedings of the Sixth SPE-Symposium on Reservoir Simulation*. New Orleans, Louisiana: Society of Petroleum Engineers. 1982.

Seth, M.S. and M. Hanano. "An Efficient Procedure for Multiple Interacting Continua Flow." *Proceeding of the World Geothermal Congress*. Florence, Italy. 1995.

Somerton, W.H., A.H. El-Shaarani, and S.M. Mobarak. "High Temperature Behavior of Rocks Associated with Geothermal-Type Reservoirs." Paper SPE-4897. *Proceedings of the 44th Annual California Regional Meeting of the Society of Petroleum Engineers*. Richardson, Texas: Society of Petroleum Engineers. 1974.

van Genuchten, M.T. "A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils." *Soil Science Society of American Journal*. Vol. 44. pp. 892-898. 1980.

GEM

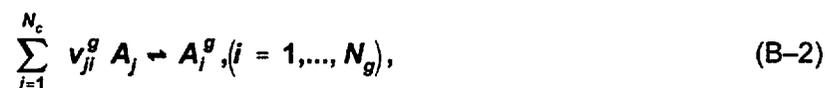
This appendix provides a brief mathematical description of the underlying equations solved by GEM for IDIF = 0 corresponding to equal solute diffusion coefficients and no electrochemical reactions. For a description of the equations solved for IDIF = 1 and 2, see Lichtner (1994).

B.1 CHEMICAL REACTIONS

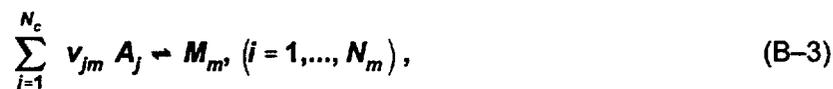
The approach used by GEM is to assume that the various chemical reactions taking place in a geochemical system can be written in terms of a basic set of independent species, or components, referred to as primary species and denoted by the set $\{A_j | j = 1, \dots, N_c\}$ (Lichtner, 1985). Generally, $N_c = N - N_R$, where N denotes the total number of chemical constituents or species, and N_R refers to the number of linearly independent reactions being considered to describe the system. The resulting reactions for aqueous, gaseous, and mineral species can be expressed in the following canonical form (Lichtner, 1985) for aqueous species A_i^l .



gaseous species A_i^g .



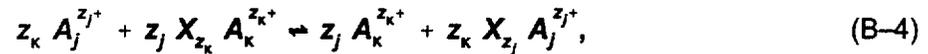
and minerals M_m



assumed to occur in numbers N_l , N_g , and N_m , respectively. The matrices v_{ji}^l , v_{ji}^g , and v_{jm} denote the stoichiometric reaction coefficients giving the number of moles of the j th primary species in one mole of the i th aqueous or gaseous secondary species and m th mineral, respectively. Each reaction is associated with a single species on the right-hand side which appears with unit stoichiometric coefficient, referred to as a secondary species. A species is distinguished by its chemical formula and the phase to which it belongs. Reactions (B-1) and (B-2) are considered to be reversible, and hence, the concentrations of the product species appearing on the right hand side are related algebraically to the concentrations of the primary species through mass

action equations [see Eqs. (B-15) and (B-17)] representing conditions of local equilibrium. The rates of these reactions are thus determined by the rate of transport within the aqueous and gas phases. Note that all gaseous species are secondary species. Mineral reactions are considered to be irreversible, their rates described by a kinetic rate law [see Eq. (B-25)]. Local equilibrium is achieved by taking the rate constant sufficiently large.

Ion-exchange reactions are assumed to be expressible in the form



for exchange of the j th and k th cations, where X denotes a surface site, and $X_{z_j} A_j$ an adsorbed species.

The species water in the aqueous phase [$\text{H}_2\text{O}_{(l)}$] is always chosen as a primary species. The remaining primary species may be any independent set of species which conveniently characterize the chemical properties of the system under investigation. In what follows, they are chosen to be a subset of the aqueous species. It is perhaps important to note that considerations with regard to the dominance of certain species over others is not essential in the choice of primary species, and any set of species, only so long as they are independent, may be used. Because of the large spatial (and temporal) variation in concentration that is possible, by many orders of magnitude for some species, it is generally necessary to solve for the logarithm of the concentration, rather than the concentration itself. This also ensures that the concentration is a positive quantity.

B.1.1 Multiphase-Multicomponent Mass Transport Equations

The transport equations solved by GEM for primary species are given by (Lichtner, 1996)

$$\frac{\partial}{\partial t} (\phi \psi_j + \bar{C}_j) + \nabla \cdot \Omega_j = - \sum_{m=1}^{N_m} v_{jm} I_m, \quad (\text{B-5})$$

where \bar{C}_j denotes the adsorbed concentration of the j th primary species, and the generalized concentration ψ_j and flux Ω_j are defined by

$$\psi_j = s_l \psi_j^l + s_g \psi_j^g, \quad (\text{B-6})$$

and

$$\Omega_j = \Omega_j^l + \Omega_j^g, \quad (\text{B-7})$$

with

$$\Psi_j^\pi = \delta_{\pi j} C_j^\pi + \sum_{i=1}^{N_\pi} v_{ji}^\pi C_i^\pi \quad (\text{B-8})$$

and

$$\Omega_j^\pi = \delta_{\pi j} J_j^\pi + \sum_{i=1}^{N_\pi} v_{ji}^\pi J_i^\pi, \quad (\text{B-9})$$

with $\pi = l, g$. The delta function appears in Eq. (B-9) because all gas species are taken as secondary species. The mineral mass transfer equation is given by

$$\frac{\partial \Phi_m}{\partial t} = \bar{V}_m I_m, \quad (\text{B-10})$$

The rate of reaction is denoted by I_m corresponding to mineral precipitation/dissolution. Here C_i^π and J_i^π denote the concentration and flux of the i th species in the π th phase, Φ_m and \bar{V}_m denote the volume fraction and molar volume, respectively, of the m th mineral. The liquid flux J_i^l appearing in these equations is defined by

$$J_i^l = -\phi \tau s_l D_l \nabla C_i^l + q_l C_i^l \quad (\text{B-11})$$

and the gas flux J_i^g by the equation

$$J_i^g = -\phi \tau s_g D_g \nabla C_i^g + q_g C_i^g, \quad (\text{B-12})$$

where D_π denotes the diffusion coefficient in phase π and q_π the velocity of phase π defined by Darcy's law as:

$$q_\pi = -\frac{k k_{r\pi}}{\mu_\pi} \nabla (P_\pi - \rho_\pi g z), \quad (\text{B-13})$$

where k refers to the saturated permeability of the porous medium, $k_{r\pi}$ represents the relative permeability, and μ_π the viscosity of phase π , g denotes the acceleration of gravity, and z points in the direction of gravity. The diffusion coefficients for aqueous species are taken to be the same for all species. For species-independent diffusivities, the flux Ω_j simplifies to the expression

$$\Omega_j^\pi = (-\phi \tau s_\pi D_\pi + q_\pi) \psi_j^\pi, \quad (\text{B-14})$$

involving directly the generalized concentration ψ_j^π

The quantities ψ_j^π and Ω_j^π may be interpreted, generally, as the total concentration and flux of the j th primary species in the liquid and gas phases provided the coefficients V_{ji}^π are positive (Lichtner, 1985). For reactions involving the hydrogen ion or redox reactions, ψ_j^π may also become negative.

These equations are completely general and include both the solvent and solute species, and gaseous species. Solving the primary species mass conservation equations provides not only the concentrations of both primary and secondary species, but also the mineral reaction rates. Combined with mineral mass transfer equations, an energy balance equation, constitutive relations for rock properties, kinetic rate laws and mass action relations, and finally initial and boundary conditions, they completely describe the system.

B.1.2 Constitutive Relations

B.1.2.1 Mass Action Equations

Constitutive relations are required for the concentrations of secondary aqueous and gaseous species. The concentration of aqueous secondary species are given by

$$c_i' = \rho_i^{\alpha-1} (y_i')^{-1} K_i' \prod_{j=1}^{N_c} (y_j' c_j')^{\nu_j}, \quad (\text{B-15})$$

where γ_i' denotes the activity coefficient, K_i' the equilibrium constant, and the quantity α providing a density correction from molality to molarity units, is defined by

$$\alpha = \rho_i^{\sum_j \nu_j \nu_j^{\prime\prime}}, \quad (\text{B-16})$$

The concentrations of gaseous species are given by

$$C_i^g = \frac{K_i^g}{RT} \prod_{j=1}^{N_c} (\nu_j' C_j')^{\nu_j^g}, \quad (\text{B-17})$$

The exchange isotherm \bar{C}_κ , with units of moles per bulk volume, is expressed in terms of the concentrations of the primary species using the mass action equations for the exchange reactions which has the form, neglecting activity coefficient corrections,

$$K_{j\kappa} = \left[\frac{C_\kappa'}{\bar{C}_\kappa} \right]^{z_j} \left[\frac{\bar{C}_j}{C_j'} \right]^{z_\kappa}, \quad (\text{B-18})$$

consistent with Eq. (B-4), where the quantities $K_{j\kappa}$ represent selectivity coefficients. Combining this relation with the site conservation equation

$$\omega = (1 - \phi) \rho_{\text{solid}} Q = \sum_j z_j \bar{C}_j, \quad (\text{B-19})$$

where Q denotes the cation exchange capacity, yields a single nonlinear equation for the j th sorption isotherm \bar{C}_j

$$\omega = z_j \bar{C}_j + \sum_{\kappa \neq j} C_\kappa' K_{j\kappa}^{1/z_\kappa} \left[\frac{\bar{C}_j}{C_j'} \right]^{z_j/z_\kappa} \quad (\text{B-20})$$

This equation implicitly defines the sorption isotherm as a function of the primary species concentrations.

The equilibrium constants K_i^π in general, are functions of temperature and pressure. An extensive database is included with the program covering a temperature range of 0–300° C along the saturation curve of water based on the EQ3/6 database (Wolery, 1992). Log values are stored at temperatures of 0, 25, 60, 100, 150, 200, 250, and 300°C and interpolated according to the Mayer-Kelly expression

$$\log K(T) = \frac{a_{-2}}{T^2} + \frac{a_{-1}}{T} + a_0 \ln T + a_1 + a_2 T, \quad (\text{B-21})$$

where T denotes the absolute temperature in degrees Kelvin. Pressure lies along the steam saturation curve for temperatures above 100 °C, otherwise it is set at 1 bar. Other databases may be generated for any desired temperature range and pressure using the computer code SUPCRT (Johnson, et al., 1992). Because of the small variation in pressure, this is considered an adequate approximation. The density of pure water is determined using the equation of state provided by Haar, et al. (1980) in uncoupled mode.

B.1.2.2 Kinetic Rate Law

Mineral reactions are assumed to be irreversible, with their rates of reaction described through a kinetic rate law. For simplicity and because of lack of knowledge of detailed reaction mechanisms, mineral reactions are represented by an overall reaction between the solid and aqueous solution. The form of the reaction rate is based on transition state theory. Precipitation or dissolution may occur depending on the sign of the affinity A_m of the reaction, defined by

$$A_m = -RT \ln K_m Q_m, \quad (\text{B-22})$$

where K_m denotes the corresponding equilibrium constant for the mineral reaction as written in Eq. (B-3), and Q_m the ion activity product, defined by

$$Q_m = \prod_{j=1}^{N_c} (\gamma_j' C_j')^{v_{jm}}, \quad (\text{B-23})$$

with R the gas constant, and T the temperature. At equilibrium the affinity and the rate vanish. The expression for the reaction rate must take into account the moving boundary nature of the transport—reaction problem. This can be accomplished with the form

$$I_m = \begin{cases} \hat{I}_m, & \Phi_m > 0 \text{ or } A_m < 0, \\ 0, & \text{otherwise} \end{cases} \quad (\text{B-24})$$

The rate \hat{I}_m is defined as the sum over a set of parallel reactions which are linearly-dependent with Eq. (B-3) as

$$\hat{I}_m = -s_m \left(\sum_l P_{ml} \kappa_{ml} \right) \left[1 - (K_m Q_m)^{\sigma_m} \right], \quad (\text{B-25})$$

where the prefactor P_{ml} is defined as

$$P_{ml} = \prod_{j=1}^{N_c} a_j^{\alpha_{jl}^m} \prod_{i=1}^{N_{cx}} a_i^{\alpha_{il}^m}, \quad (\text{B-26})$$

κ_{ml} denotes the kinetic rate constant for the l th parallel reaction, s_m denotes the specific mineral surface area participating in the reaction, σ_m denotes Temppkin's constant a_i represents the activity of the i th species, and $\alpha_{jl}^m, \alpha_{il}^m$ are constants. With this form of the rate, the effective kinetic rate constant κ_m may be pH-dependent with the form

$$\kappa_m = \kappa_m^a a_{H^+}^{\beta a} + \kappa_m^b a_{H^+}^{\beta b} + \kappa_m^0, \quad (\text{B-27})$$

for example, by choosing appropriate prefactors and rate constants in the sum in Eq. (B-25).

A transport-limited form of the rate law can be devised according to the expression

$$\hat{I}_m = -s_m \sum_l P_{ml} \kappa_{ml} \left[\frac{1 - (K_m Q_m)^{\sigma_m}}{1 + \frac{P_{ml} \kappa_{ml} (K_m Q_m)^{\sigma_m}}{r_{lim}}} \right] \quad (\text{B-28})$$

with transport-limited rate r_{lim} . For $Q_m \rightarrow \infty$,

$$\hat{i}_m \rightarrow N_m^p r_{lim} \quad (\text{B-29})$$

with N_m^p the number of parallel reactions.

In GEM the surface area s_m is expressed relative to the bulk volume of an REV with units of cm^{-1} . Mineral surface area may be expressed in a variety of different ways depending on the reference volume chosen. The relationship between surface area expressed relative to a REV volume and mass of fluid is given by

$$s_m^v = \phi \rho f s_m^M, \quad (\text{B-30})$$

where s_m^v refers to the REV volume-based surface areas, s_m^M refers to the surface area based on mass of fluid (usually taken as 1 kg H_2O), ρf denotes the fluid density in the appropriate units [kg cm^{-3}], and ϕ denotes the porosity. Grain size b_m and surface area can be correlated using the phenomenological relationship

$$s_m^v = \frac{6}{b_m} \phi_m, \quad (\text{B-31})$$

where the factor six comes from the six sides of a cube.

The reaction rate has units of moles per unit time per unit volume of bulk porous medium and is taken as positive for precipitation and negative for dissolution. Thus, it represents an average rate taken over a representative elemental volume (REV). This form of the rate also includes overall oxidation/reduction reactions in which electron transfer is not represented explicitly. The rate law given by Eq. (B-25) should really be referred to as a pseudo-kinetic rate law. Because it refers to the overall mineral precipitation/dissolution reaction, it generally does not describe the actual kinetic mechanism by which the mineral reacts. Nevertheless, it provides a useful form to describe departures from equilibrium. Close to equilibrium the rate becomes proportional to the chemical affinity.

The temperature dependence of the kinetic rate constants is calculated through the expression:

$$\kappa_m(T) = \kappa_m^0 \frac{T}{T_0} \exp \left[- \left(\frac{1}{T} - \frac{1}{T_0} \right) \frac{\Delta H_m^\ddagger}{R} \right], \quad (\text{B-32})$$

where k_m^0 denotes the rate constant at reference temperature T_0 and ΔH_m^\ddagger denotes the enthalpy of activation.

For kinetic homogeneous aqueous reactions a rate law of the form

$$I_j = - \left(\sum_I P_{jI} \kappa_{jI} \right) [1 - K_j Q_j], \quad (\text{B-33})$$

and an analogous transport-limited form

$$I_j = - \sum_I P_{jI} \kappa_{jI} \left[\frac{1 - K_j Q_j}{1 + \frac{P_{jI} \kappa_{jI} K_j Q_j}{r_{\text{lim}}}} \right], \quad (\text{B-34})$$

is used. The ion activity product Q_j is defined as

$$Q_j = (a_j^I)^{-1} \prod_{j'=1}^{N_c} (\gamma_{j'}^I c_{j'}^I)^{\nu_{j'}^I}, \quad (\text{B-35})$$

where a_j^I denotes the activity of the j th aqueous primary species.

B.1.2.3 Porosity-Permeability Coupling

Porosity and mineral volume fractions are related by the equation

$$\phi = 1 - \sum_{m=1}^{N_m} \phi_m. \quad (\text{B-36})$$

However, this expression is not completely general and may be deceptively simple because no distinction is made between connected and total porosity, which includes deadend porosity. By relating the permeability and tortuosity to porosity through various phenomenological relations, it is possible to couple changes in porosity to the flow field and transport of solutes. One such relation is the power law expression of the form

$$\kappa = \kappa_0 \left(\frac{\phi}{\phi_0} \right)^n, \quad (\text{B-37})$$

where k_0 and ϕ_0 denote the initial permeability and porosity where n is a real number. The tortuosity can be represented by a similar relation

$$\tau = \tau_0 \left(\frac{\phi}{\phi_0} \right)^n, \quad (\text{B-38})$$

where τ_0 denotes the initial tortuosity

Because of the possibility of the porosity becoming close to zero (a lower cutoff value of 10^{-10} is used to prevent the porosity from becoming exactly zero or negative), special care is required to ensure that mineral surface areas also tend to zero as all available pore volume at any point becomes completely filled with secondary alteration products. Failure to account for reduction in surface area would result in prohibitively small time steps. To accomplish this, a phenomenological relation for the surface area is used of the form

$$s_m = s_m^0 \left(\frac{\phi \phi_m}{\phi_0 \phi_m^0} \right)^{2/3}, \quad (\text{B-39})$$

for primary minerals ($\phi_m^0 > 0$), and

$$s_m = s_m^0 \left(\frac{\phi}{\phi_0} \right)^{2/3}, \quad (\text{B-40})$$

for secondary minerals ($\phi_m^0 > 0$). The porosity factor which appears in both expressions assures that the surface area becomes zero as the porosity vanishes. It should be noted that there is no rigorous justification for these relations. In particular, the $2/3$ power is based on a simple geometric relation of surface area on volume. A capillary tube model might result in a square root behavior, for example.

According to the expression for the primary mineral surface area, the surface area decreases as the mineral dissolves. While this must indeed be the case as the mineral approaches complete dissolution, it need not necessarily apply during intermediate time periods when etch pits form possibly increasing the surface area.

B.2 NUMERICAL SOLUTION

Several different options are available for solving the transport equations. The implicit approach is generally superior for one-dimensional problems. However, for two- and three-dimensional problems, explicit or operator-splitting algorithms may be necessary, especially for large numbers of species and grid points.

An explicit method is used to solve the mineral mass transfer equations given by:

$$\varphi_m(r, t + \Delta t) = \varphi_m(r, t) + \Delta t \bar{V}_m I_m(r, t), \quad (\text{B-41})$$

where the mineral reaction rate $I_m(r, t)$ is taken from the previous time step. The time step size Δt depends on how close the solution to the aqueous and gaseous species transport equations is to a stationary state (Lichtner, 1988). For the transient case, the same time step Δt is used as in the transient transport equations. When the system has reached a stationary state, however, a much larger time step can be taken without fear of violating the stability conditions. In this case, the time step size is only restricted by the maximum absolute change allowed in the mineral volume fraction. The allowable time step size is also controlled by limiting the negative most value of the mineral volume fraction to an acceptable value which may be taken as zero. Note, however, that at a reaction front where the mineral volume fraction vanishes, according to Eq. (B-41) in order for the front to move, the volume fraction must become negative over some region surrounding the front. This is, of course, nonphysical and the volume fraction must be set back to zero to eliminate the negative values, if they occur.

In the transient regime, the change in mineral abundances and, hence, porosity and permeability, is generally much slower than the change in aqueous and gaseous compositions as well as temperature, pressure, and saturation. The time evolution of the system can be divided into a sequence of transient and stationary state regimes. The term stationary is preferred to the term steady to distinguish this situation from that of constant velocity. When the fluid compositions become stationary in time, a much larger time step can be taken compared to the transient regime. As minerals dissolve and precipitate and reaction fronts move to new locations, the system reverts again to a transient regime until a new stationary state is established. In this way the time evolution of the system is represented as a sequence of stationary states separated by transient intervals.

B.2.1 Sequentially Coupled Two-Phase Flow and Transport

A sequentially coupled methodology is used to solve the multidimensional, multiphase, multicomponent fluid and solute flow and transport equations in a partially saturated porous medium. In this approach, heat, air and water vapor, 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 changes in 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 used involves different strategies depending on the dimensionality of the problem. For one-dimensional systems a fully implicit time-stepping algorithm with dynamically computed adaptive time steps is recommended to solve both the heat and solvent transport equations, and the geochemical reactive transport equations. For large two- and three-dimensional problems, an operator-splitting algorithm is preferred in which flow and transport time steps are decoupled from the chemical algorithm.

Field variables are linearly interpolated over a METRA time step. Thus, for some field variable $F(t)$

$$F(t') = \left(1 - \frac{t' - t}{\Delta t}\right) F(t) + \left(\frac{t' - t}{\Delta T}\right) F(t + \Delta t), \quad (\text{B-42})$$

where F represents the flow velocity, saturation, pressure, and temperature calculated from METRA, t and $t + \Delta t$ denote METRA time steps, and t' the desired interpolation time, with $t \leq t' \leq t + \Delta t$.

B.2.2 Implicit Finite Difference

The transport equations are solved using an implicit finite difference scheme. Finite difference formulations include first order upwinding and the hybrid scheme of Patankar (1980) which uses first-order upwinding or central differencing depending on the value of the local grid Peclet number. Several different solver options are available for inverting the sparse Jacobian matrix. For one-dimensional problems, a block tri-diagonal solver is used. For two- and three-dimensional problems, an iterative solver WATSOLV is used (van der Kwaak, et al., 1995).

B.2.3 Operator Splitting

Operator splitting is a powerful numerical technique for solving large two- and three-dimensional systems involving a number of chemical species with multiple time scales,

with distinct advantages over the conventional fully implicit formulations. The advantages lie primarily in the area of computational efficiency, both in terms of the execution speed and the memory requirements. For large systems with tens of thousands grid blocks and dozens of species, operator splitting may reduce the computing time by factors of ten in some cases. This advantage is progressively less significant for smaller systems with a fewer species.

In operator splitting methods, the integration process is split into two (three in case of Strang Splitting) steps, namely a transport step, followed by a reactive step such that the transport and the reactive terms are solved independently of each other. Furthermore, in the transport step each phase and each species are solved sequentially one at a time. The solution obtained during the transport step is used as the initial condition for the reactive step. Thus, the procedure neglects any coupling or interaction between the transport and the reaction rate. While the method preserves the mass balance for each of the components, it introduces errors associated with the effect of unaccounted coupling between the transport and the reaction. In effect, the method assumes that reaction rate is unaltered by the transport step. This is a reasonable assumption for low rates and/or small time step sizes. It should be noted that the splitting errors are in addition to the errors introduced due to discretization and other numerical approximations.

Since time scales for reactions are vastly different, the solution for the reaction rate is obtained (if necessary) by taking several steps within a transport step. Each successive step uses the solution obtained during the preceding substep.

Of several possible implementations of operator splitting technique, GEM employs two of the commonly used formulations and two novel variants as outlined below.

B.2.3.1 Conventional Operator Splitting Procedure

Step (1) The nonreactive transport equations for gaseous and aqueous species are solved independently of each other over a single time step to provide the total concentrations $\tilde{\psi}_j^l(r, t + \Delta t)$ and $\tilde{\psi}_j^g(r, t + \Delta t)$ where the tilde (~) indicates nonreactive transport and l (g) refers to liquid (gas). The nonreactive transport equations for aqueous and gaseous species read:

$$\frac{\partial}{\partial t} (\phi s_{\pi} \tilde{\psi}_j^{\pi}) + \nabla \cdot \tilde{\Omega}_j^{\pi} = 0, \quad (\text{B-43})$$

where $\pi = l, g$.

The above equations are solved with liquid phase implicit (IOPS = 1) or explicit (IOPS = 0). The gas phase is always treated implicitly due to substantially higher gas velocity. The specified boundary conditions and source/sinks are imposed during this step.

Step (2) Reaction step in which the reaction path equations for dissolution and precipitation of minerals are solved over a single time step using total concentrations obtained from the nonreactive step. At each node, the mass transfer equation

$$\frac{\partial}{\partial t} [\varphi(s_l \psi_j^l + s_g \psi_j^g)] = - \sum_m v_{jm} I_m, \quad (\text{B-44})$$

is solved, subject to the initial condition

$$\psi_j^\pi(r, t) = \tilde{\psi}_j^\pi(r, t + \Delta t), (\pi = l, g) \quad (\text{B-45})$$

with $\tilde{\psi}_j^\pi(r, t + \Delta t)$ obtained from the non-reactive step. Eq. (B-44) is solved implicitly. Since these equations involve no interblock coupling due to transport, they can be solved block by block. The final solution is taken as the desired solution. Note that no sources/sinks or boundary conditions are specified in this step.

B.2.3.2 Strang Splitting

This is a three step procedure where first the (i) transport is solved for a step size of $\Delta t / 2$, followed by a (ii) reactive step of size Δt , and finally, the (iii) transport step again with a step size of $\Delta t / 2$. In each step, solution obtained in the preceding step is used as the initial condition for the following step.

The equations are very similar to the preceding method, and are repeated here for clarity. The transport step over the time step $\Delta t / 2$ is

$$\frac{\partial}{\partial t} (\varphi s_\pi \tilde{\psi}_j^\pi) + \nabla \cdot \tilde{\Omega}_j^\pi = 0, \quad (\pi = l, g) \quad (\text{B-46})$$

which is followed by the reactive step

$$\frac{\partial}{\partial t} [\varphi(s_l \hat{\psi}_j^l + s_g \hat{\psi}_j^g)] = - \sum_m v_{jm} I_m, \quad (\text{B-47})$$

subject to initial conditions

$$\hat{\psi}_j^\pi(r, t) = \tilde{\psi}_j^\pi\left(r, t + \frac{\Delta t}{2}\right), \quad (\pi = l, g) \quad (\text{B-48})$$

The final transport step uses this total concentration as an initial condition to obtain the desired concentration at time :

$$\frac{\partial}{\partial t} (\varphi s_\pi \psi_j^\pi) + \nabla \cdot \Omega_j^\pi = 0, \quad (\pi = l, g) \quad (\text{B-49})$$

$$\psi_j^\pi\left(r, t + \frac{\Delta t}{2}\right) = \hat{\psi}_j^\pi(r, t + \Delta t), \quad (\pi = l, g) \quad (\text{B-50})$$

Strang method (IOPS = 2) uses only implicit option for transport. Strang's algorithm is second order accurate in splitting errors as opposed to the first order accuracy of the preceding method.

B.2.3.3 Inclusion of Boundary Condition in the Reactive Step

In the conventional operator splitting procedure, the effect of boundary condition is ignored in the reactive step. Since the boundary flux terms only modifies the diagonal terms, it can be readily incorporated into the reactive step. This, in effect, accounts for the flux due to a change in the concentration due to reactions. Inclusion of it in a test problem involving a single component quartz system dramatically improved the results as should be expected. Additional testing is warranted for this option.

B.2.3.4 Inclusion of Reaction Rate in the Transport Step

In this procedure, the reaction rate is introduced in the transport step explicitly based on the value at the beginning of a time step. The rate imposed is subtracted during the reactive step. This should result in a reduced splitting error. A weight factor may be used to allocate the rate during the two steps. GEM uses the weight factor *wtkin* (see OPTS keyword).

B.2.4 Implicit Rate Explicit Transport (ImRET)

In a fully implicit formulation, the off diagonal terms in the Jacobian matrix arise from velocity and the diffusion processes. Thus, if the velocity and the diffusion coefficients are small, these off-diagonal terms may be ignored without impairing the numerical stability, thus offering substantial savings in the computing time and the memory requirements. All interblock couplings are eliminated by such treatment, and the solution can be obtained one block at a time. This is implemented in GEM and can be invoked as METHOD = 3 (see OPTS keyword). Limited tests with a 12 component copper leaching problem showed a substantial reduction in the computing time. Note that ignoring the off-diagonal Jacobian coefficients does not result in any loss of accuracy; however, the number of Newton iterations is likely to increase.

B.3 REFERENCES

- Haar, L., J.S. Gallagher, and G.S. Kell. "Thermodynamic Properties of Fluid Water." *Water and Steam: Their Properties and Current Industrial Applications*. J. Straub and K. Scheffler, eds. New York City, New York: Pergamon Press. pp. 69–82. 1980.
- Johnson, J.W., E.H. Oelkers, and H.C. Helgeson. "SUPCRT92: A Software Package for Calculating the Standard Molal Thermodynamic Properties of Minerals, Gases, Aqueous Species, and Reactions from 1 to 5000 Bars and 0 °C to 1000 °C." *Computers and Geosciences*. 1992.
- Lichtner, P.C. "Continuum Model for Simultaneous Chemical Reactions and Mass Transport in Hydrothermal Systems." *Geochimica et Cosmochimica Acta*. Vol. 49. pp. 779–800. 1985.
- Lichtner, P.C. "The Quasi-Stationary State Approximation to Coupled Mass Transport and Fluid-Rock Interaction in a Porous Medium." *Geochimica et Cosmochimica Acta*. Vol. 52. pp. 143–165. 1988.
- Lichtner, P.C. "Time-Space Continuum Description of Fluid/Rock Interaction in Permeable Media." *Water Resources Research*. Vol. 8, No. 12. pp. 3,135–3,155. 1992.
- Lichtner, P.C. "Engineered Barrier System Performance Assessment Codes (EBSPAC) Progress Report October 1, 1993, through September 25, 1994." CNWRA 94-026. San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. 1994.
- Lichtner, P.C. "Continuum Formulation of Reactive Transport." Reactive Transport in Porous Media. P.C. Lichtner, C.I. Steefel, and E.H. Oelkers, eds. *Reviews in Mineralogy*. Vol. 34. pp. 1–81. 1996.
- Pantakar, S.V. Numerical heat transfer and fluid flow. New York, NY: Hemisphere Corporation: 197. 1980.
- van der Kwaak, J.E., P.A. Forsyth, and E.A. Sudicky. WATSOLV, Sparse Matrix Iterative Solver Package, User's Guide. Waterloo, Ontario, Canada: Waterloo Centre for Groundwater Research, University of Waterloo. 1995.
- Wolery, J.J. EQ3NR, A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations: Theoretical Manuals, User's Guide, and Related Documentation. Version 7.0. UCRL-MA-110662 PT III. Livermore, California: Lawrence Livermore National Laboratory. 1992.

MULTIFLO USER'S MANUAL

**TWO-PHASE
NONISOTHERMAL
COUPLED THERMAL-
HYDROLOGIC-CHEMICAL
FLOW SIMULATOR**

Prepared for

**U.S. Nuclear Regulatory
Commission**

Prepared by

**Center for Nuclear Waste
Regulatory Analyses
San Antonio, Texas**



**MULTIFLO USER'S MANUAL
TWO-PHASE NONISOTHERMAL COUPLED
THERMAL-HYDROLOGIC-CHEMICAL
FLOW SIMULATOR**

Prepared for

**U.S. Nuclear Regulatory Commission
Contract NRC-02-97-009**

Prepared by

**Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas**

