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

Prepared for

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

Prepared by

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

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MULTIFLO VERSION 2.0

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*The original version of this document and the early versions of the MULTIFLO code were principally authored by Dr. Peter Lichtner while he was a member of the staff at the Center for Nuclear Waste Regulatory Analyses. Dr. Lichtner is currently at the Los Alamos National Laboratory, Los Alamos, New Mexico. The authors of this revision gratefully acknowledge Dr. Lichtner's contribution.

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: No data is presented in this report.

ANALYSES AND CODES: This computer code has been developed under the CNWRA Software Configuration Procedures described in TOP–018. This controlled MULTIFLO Version 2.0 replaces Version 1.5, which was released December 2001. Information on development of this code is available in Scientific Notebook #282E and the MULTIFLO Software Development file.

1 INTRODUCTION

The computer code MULTIFLO was developed to aid in understanding perturbations to the near-field environment surrounding a proposed 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 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 high-level waste disposal site proposed for 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 1.5, which was released in December 2001. 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 1.5 to version 2.0. In particular, several changes were made to improve code stability and ease of use, and new capabilities to describe groundwater pumping wells were added. In addition, several errors in the manual were corrected. A small number of coding errors were also uncovered and detected as part of the ongoing testing process. These coding errors affected code stability; no results published in previous reports or journal articles were affected.

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 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. Media 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. Energy transfer by thermal radiation is also an option. Arbitrary user-specified spatial variation in porosity, absolute permeability (in all three spatial directions), tortuosity, thermal conductivity, 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	p_l, X_a, T
Two-phase	p_g, p_a, s_g
Single-phase gas	p_g, p_a, T

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 Dirichlet (constant field variables), Neumann (constant flux), and mixed 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 and energy balances are calculated based on cumulative and incremental balances to monitor the accuracy of the solution. Mass transfer in the gas phase includes enhanced binary diffusion. Extensive default parameters are provided for properties of air, convergence criteria, method of solution, and diffusion parameters. Pressure-volume-temperature properties for H_2O are calculated optionally by a rapid table look-up procedure or by using the International Formulation Committee (1967) functions. Vapor-liquid equilibria may be defined with lowered vapor pressure resulting from capillary forces. 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 Brooks-Corey 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 and other thermodynamic variables for the matrix equal 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

The active fracture model (Liu, et al., 1998) may be implemented using the dual continuum model with appropriately defined tables for saturation dependent properties. 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 blocks 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.

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.

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–1)].

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
= 2, GEM stand-alone
= 3, Coupled METRA and GEM in transient mode
= 4, METRA 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, initial porosity, temperature, pressure, and saturation are taken from METRA.

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 has also been run on HP workstations, and on an Apple IMAC with the Mac OS X operating system using a public domain compiler. Version 2.0 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, 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 start time keyword as below.

2.2.1.2 Start Time Keyword

This keyword sets the time at the beginning of a run. A normal run starts from time = 0, whereas, a restart run starts from time > 0.

Read:	RSTARt NRST TIME
RSTARt	Keyword defining start time.
NRST	Not used.
TIME	Start time [s] for the simulation.

Example: Fixed Data

```
This is a test run for a 3D dual continuum system
  April 10, 1998
:
RSTARt 0 0.0 :normal run

RSTARt 0 3.5e7 :restart run starting after 3.5 × 10^7 seconds.
```

Comment(s):

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

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	
EQUIlibration	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	
WBC	Optional	
WBHP	Optional	
WELLS	Optional	
WRATe	Optional	
WREComp	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 CO_2, 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 H_2O.

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 (CO_2) 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.

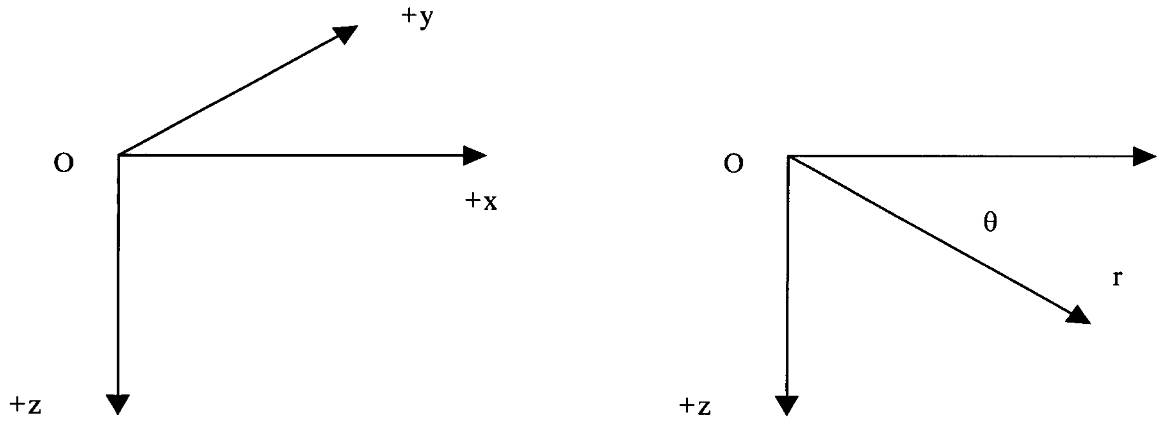

Figure 2-1. Coordinate Systems Used for Cartesian and Radial Geometries

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:
                       :     igrid     rw     re
                       CXYZ   0        0      0
```

```
Cartesian Geometry:
   :     igrid       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:
         igrid 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 FMFAC

Structured Grid Read: I1 I2 J1 J2 K1 K2 SIGMAF AREAMOD XLM YLM ZLM FMFAC

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.
FMFAC	Fracture-to-matrix relative permeability factor. If FMFAC>0, the relative permeability for fracture-to-matrix flow is adjusted by the multiplier FMFAC. If FMFAC is a negative integer, then the relative permeability curve designated |FMFAC | in the PCKR keyword is used for fracture-to-matrix flow. Matrix-to-fracture flow is unaffected by FMFAC.

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 active fracture model of Liu, et al. (1998) can be invoked by setting FMFAC to a negative integer and using the tabular option in the PCKR keyword.

Examples:

```
DCMParameters
1  3   1  1  1  5  0.01  1.0e-3  .1  .1  .1
/

DCMParameters
1  10  1  10  1  10  0.01  1.  .1  .1  .1  -5
```

2.2.2.6 Depths of Grid Blocks [DEPTh]

Initialization Data

Keyword: **DEPTh**

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: DEPTh IDEPTH DIP

DEPTh 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,..., 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,..., 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,..., 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*(θ)-, 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

IPVCAL 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 H_2O 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 [°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 NX = NY = 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 IPVCAL = 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 5–369 °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 × 1 × 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*(*θ*)-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 [°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 Slipage 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 [m^2].

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*(θ)-, and *z*-directions to calculate BKLINT using a log(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:

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

where

$$b = \mathrm{BKLINT}\ [\mathrm{Pa}] \tag{2-2}$$

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

$$K_{\mathrm{abs}} = \text{absolute rock permeability } [\mathrm{m}^2] \tag{2-4}$$

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/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 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_{rl} = 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 dPcw/dSw 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 Pc/Kr 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(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.
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 KRW = 0 at or below SWIRM liquid saturation and KRG = 0 at or above (1-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
fkrg=(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
```

2.2.2.14 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	$x(r)$-directional absolute rock permeability [m^2].
PERMY	$y(\theta)$-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

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

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

$$\phi_n = \frac{\kappa_n}{\kappa}\overline{\phi} \tag{2-6}$$

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
```

2.2.2.15 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/m^3].
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 [m^2/s] [see Eq. (A–16)] (default = 2.13e-5 m^2/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
BCONdition
DEBUg
ENDS
LIMIt
OUTPut
PLOTs
RECUrrent
RSTARt
SOLVe
SOURce
STEAdy
TIME
TOLR
WBC
WBHP
WELLs
WRAT
WREC

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 **= 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  facl
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.

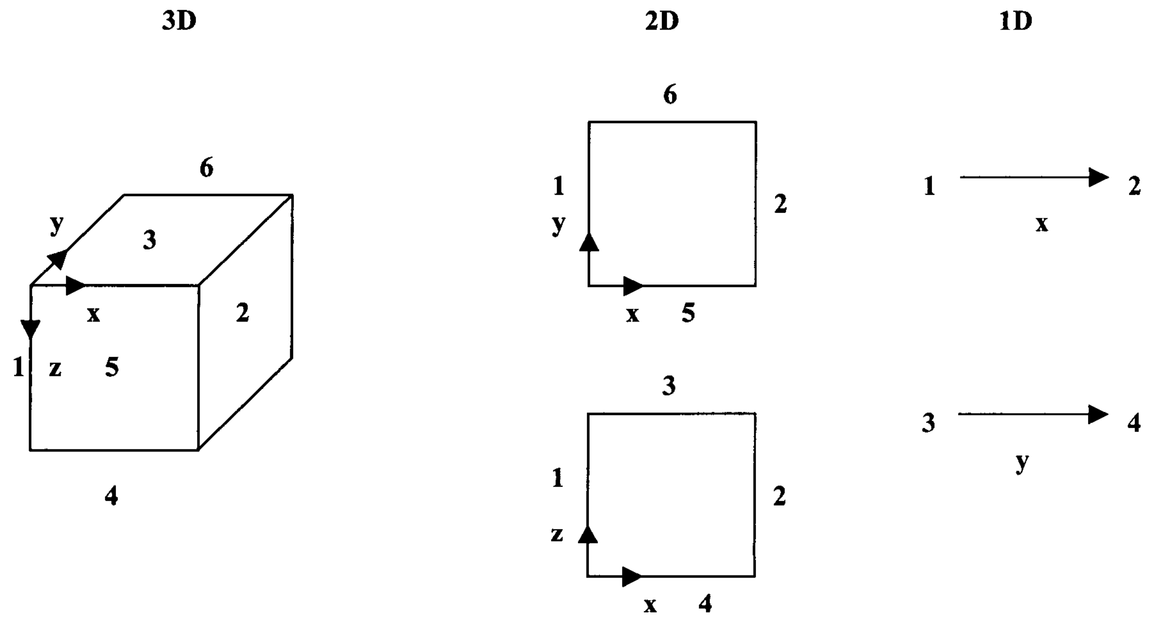

Figure 2-2. Boundaries of Computational Domain in Cartesian Coordinates

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 XABCF 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 [m^2].
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 [kg/m^2/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 [°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, $q_{\mathrm{rad}} = \sigma$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=I 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=I (where I is an integer as defined above) is specified such that I 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.

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 [$J/m^3/s$]. 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 $J/m^3/s$ for j = 2. The units for QMT are kg/s for j = 1 and 3, and $kg/m^3/s$ 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 DTMPSTDY
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).
DTMPSTDY	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 abs(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[yrs] 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.

2.2.3.12 Wellbore Coefficient Data [WBC]

Recurrent Data Keyword: **WBC**

Optional

This keyword is required if a wellbore coefficient is to be changed for one or more wells.

A wellbore coefficient may change if the well has undergone acidization or fracturing, or has deteriorated.

Read: WBC N

Read: L WBC(1) WBC(2) WBC(3) . . WBC(NCMPW)
. . . . 10 wbc values per line

Read WBCs successively for each of the N wells.

WBC	Keyword for modifying wellbore coefficients.
L	Well identifier (see WELLs keyword).
N	Number of wells for which the WBC is to be modified.
NCMPW	Number of well completions.

Data for all N wells may be read in any order.

See keyword WELLs for more details about WBC.

Example:

```
WBC   2
1   1.e-13  2.4e-15   1.7e-13
2   1.e-13  1.e-14   1.e-12
```

2.2.3.13 Well BHP Data

Recurrent Data

Keyword: **WBHP**

Optional

This data set is required if a change is to be specified for well bottomhole pressure, and/or injection enthalpy or temperature parameters.

Read: WBHP N

Read: L BHPF TWINJ
. . . .

WBHP	Keyword for reading rate control data.
N	Number of wells to be modified.
L	Well identifier (see WELLs keyword).
BHPF	Flowing bottomhole pressure, Pa.
TINJ	Injection fluid temperature. If specified a negative value, its absolute value is assigned as the injection enthalpy.

If only one of the parameters is to be changed, leave the other as zero, and the code will retain the value assigned earlier.

Example:

```
BHP   2
7       10     0    0    0
3        0   300.   0    0
```

2.2.3.14 Injection of Extraction Wells [WELLs]

Recurrent Data

Keyword: **WELLs**

Optional

This keyword specifies grid blocks associated with injection or extraction wells. Data corresponding to this set are read once for each well when it is first introduced. Any other changes in existing wells such as rates, completion intervals, etc., are introduced by the WBHP, WREC, WRAT and WBC keywords.

Read: WELLS NW NWCMAX

Read: L WN IWTYP NWCMP IJK1 IJK2 IJK3 IJK4 IJK5

if NWCMP > 1 and the geometry is structured,

Read: IW JW KW

. . .

if NWCMP > 5 and the geometry is unstructured,

Read: ND (6) ND (7) ND (8) ND (9) ND (10) (5 Nodes/line)

. . . . .

Read: WBC (1) WBC (2) WBC (3) . . . WBC (N) (10 values/line)

. . . .

Read: Q BHP TWINJ

Repeat the above read sequence for each successive well for a total of NW wells. The wells do not have to be read in sequential order.

WELLs	Keyword for reading input data for new wells.
NW	Number of new wells introduced at this time.
NWCMAX	Maximum number of well completions (well production/injection nodes) permitted in any well. This parameter must be assigned during the first introduction of "WELL" keyword and cannot be altered, as it will be ignored in subsequent data sets for this keyword.
L	Sequential well identification number $1 < L < NW$.

WN	Any 8-character alphanumeric name for the well.
IWTYP	Index of well type.

= 11	Water injection or liquid production without any bottom hole pressure (BHP) constraint.
= 13	Same as above except constrained by BHP. If the injection pressure exceed the given maximum BHP or the flowing bottom hole pressure falls below BHP for a producing well, the rate is reduced to satisfy the constraint.
= 21	Air injection well. At present, production of air cannot be specified.
= 23	Air injection well constrained by bottomhole pressure.
= 31	Gas (air plus water vapor) injection/extraction well with no bottom hole pressure constraint.
= 33	Gas (air plus water vapor) injection/extraction well constrained by bottom hole pressure.
= 41	Total mass production rate not constrained by the specified bottomhole pressure.
= 43	Total mass production rate constrained by bottomhole flowing pressure.

NWCMP	Maximum number of blocks in which the well is to be completed at any time during the entire simulation run. If a well is completed in two nodes currently, and later these two nodes are replaced by other two different nodes, the NWCMP parameters will be 4 for this case. NWCMP = 0 for a structured grid where the well is vertical, or horizontal in a given plane parallel to I or J directions. In this case, two of the 3 coordinates (I,J,K) will remain fixed and a third one will vary defining the span of well completion nodes. NWCMP > 0 for a unstructured grid geometry, or for the case when the well is not aligned with one of the coordinate axes.
IJK1 IJK2 **IJK3 IJK4** **IJK5**	These indices designate the well completion blocks. All blocks which are now or later intersected by the wellbore must be assigned. If any of the intervening blocks are to be shut-in, simply set well bore coefficients (defined below) for these blocks to zero. In a structured geometry, IJK5 is not used.

If the well is parallel to one of the coordinate directions, (I,J, or K), two of the indices are fixed and remaining two identifies the orientation of the well (vertical, or parallel to I or J axis). For a vertical well located in I = 3, J = 5, and completed in K = 5 through 8, the indices will be read as 3 5 5 -8. The index with a negative value identifies the orientation of the well. A well parallel to I axis completed in I = 4 to 7, will be designated at 4 -7 IJK3 IJK4.

In a structured geometry, if the well is not parallel to one of the major axes, IJK4 is not used. Instead, IJK1, IJK2, IJK3 define the first well producing node. A set of NWCMP-1 additional lines must be read successively to designate all NWCMP completion nodes.

For an unstructured drift, IJK1, . . .IJK5 designates the well nodes. If NWCMP > 5 additional nodes are read successively with 5 nodes per line until all NWCMP nodes are read-in.

WBC Wellbore coefficient or well geometric factor.

Read one value for each block in which the well is completed during the entire simulation run. WBCs must be read in the same order as the well completions defined above. If at any time flow is not desired from some blocks, WBC may be set to zero for those shut-in blocks.

WBC may be approximated as:

```
2,*3.14159*k*h/ (ln)re/rw)+s-0.5)
```

re = equivalent radius of grid block

rw = radius of wellbore

s = skin factor

k*h = permeability times thickness of producing face

While a well PI (productivity index) is a function of pressure, temperature, and saturation, WBC is independent of them, and in general, will change only if the rock permeability is altered such as during hydraulic fracturing, acidization, and gradual well damage.

WBC for all well blocks must be read with 10 values/line.

Q Well rate (kg/sec). Production is negative and injection is positive.

BHP Limiting bottom-hole pressure. It is ignored if the well type is such that it is not constrained by minimum (producer) or maximum (injector) specified bottomhole pressure, Pa.

TWINJ Well injection temperature, (°C). This parameter is not used for production wells. If TWINJ is read as a negative number, its absolute value is taken as the enthalpy of injection fluid, (KJ/kgm).

It is not necessary to assign all the wells initially as some of them may become active only at a later date. However, it might be convenient to assign them initially and read a rate of zero for inactive wells.

Example:

```
WELLS   2   4
:L WN     IWTYP  NWCMP  IJK1  IJK2  IJK3  IJK4  IJK5
1 well-p   43     0      3     7     1    -4      !vert. Well completed in 1-4
1.e-14  1.e-13  1.e-12  1.e-12
-1.e-2  5.e5  120.
2  well-1  11  0  1  -3  6  6       !horizontal well parallel to I-axis in 1-3
1.e-15  2.e-12  1.e-12
1.e-1  0  50
```

2.2.3.15 Well Rates Data [WRATES]

Recurrent Data Keyword: **WRATES**

Optional

This data set is used if a change in production or injection rate is to be imposed on one or more of the wells.

Read: WRATES N

if N = 0,
read: (Q (L), L=1, NW)

if 0< N <NW,
read: L1 Q (L1)
L2 Q (L2)
. . . .
LN Q (N)

WRATES Keyword for reading changes in well rates data.

N > 0, Designated wells undergoing rate change.

= 0, All the wells are undergoing rate change (such as, the rates must be read consecutively in ascending order of well number beginning with well 1.

NW Total number of wells (injectors and producers).

Q Well rate, kg/sec. Read 10 values per line if NW > 10.

L1, L2 Sequential well numbers.

Q (L1) Q (L2) Rates for well number L1, L2, . . ., etc.

Examples:

```
RATES     3
   1    -200
   3    -500
   2    0.

RATES     0
  -0.2    -.01 .5    1.0    -1.e-2    1.5     ! Number of total wells = 6
```

2.2.3.16 Well Recompletion Data [WREComp]

Recurrent Data

Keyword: **WREComp**

Optional

This data set is required if a change in well type is desired.

Read: WRECOMP N

Read: L1 IWTYP (L1)
. . .
. . .
Ln IWTYP (Ln)

Read a total of N lines corresponding to each N wells.

WRECOMP	Keyword for changing the well type.	
N	Number of wells to be changed.	
L	Sequential well number 1 =< L <= NW	
IWTYP	**= 11**	Water injection or liquid production without any bottom hole pressure (BHP) constraint.
	= 13	Same as above except constrained by BHP. If the injection pressure exceeds the given maximum BHP or the flowing bottomhole pressure falls below BHP for a producing well, the rate is reduced to satisfy the constraint.
	= 21	Air injection well. At present, production of air cannot be specified.
	= 23	Air injection well constrained by bottomhole pressure.
	= 31	Gas (air plus water vapor) injection/extraction well with no bottomhole pressure.
	= 33	Gas (air plus water vapor) injection/extraction well constrained by bottomhole pressure.
	= 41	Total mass production rate not constrained by the specified bottomhole pressure.
	= 43	Total mass production rate constrained by bottomhole flowing pressure.

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:

$$m = i + (j - 1)\, nx + (k - 1)\, nx * ny \qquad (2\text{-}5)$$

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 `lfn_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 nonsiothermal 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 ≥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 ≥ 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 $Al(OH)_4^-$ 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).

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–33)].
NSECAQ	Number of secondary species in prefactor [see Eq. (B–33)].
RKAQ	Rate constant [moles/cm^3/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]
:itypkaq   npri nsec rk [moles/cm³/s]
:
h2(aq)      1     20
    30      1     0  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_l 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 specifies nodes at which solution compositions are printed in 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

Unstructred 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
al+3          3       1.e-4     muscovite
h+            8       6.0
sio2(aq)      3       1.e-3     quartz
hco3-         4      -2         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
al+3          3       1.e-4     muscovite
h+            8       7.0
sio2(aq)      3       1.e-3     quartz
hco3-         4      -2         co2(g)
/
k+            3       1.e-4     k-feldspar
al+3          3       1.e-4     muscovite
h+            8       7.0
sio2(aq)      3       1.e-3     uartz
hco3-         4      -2         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 [COUPle]

Initialization Data Keyword: **COUPle**

Optional

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

Read:	COUPle ISYNC IPOR IPERM PERMFAC PORFAC ICKSAT SLCUTOFF
COUPle	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

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*(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.

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.

In coupled mode DCMP parameters are taken from the METRA input file.

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 [cm^2/s].
DELHAQ	Activation enthalpy [kJ/mol].
DGAS	Gaseous diffusion coefficient [see Eq. (A–16)] [cm^2/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 [cm^2/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[cm^2/s] delhaq[kJ/mol] dgas[cm^2/s] dgexp tortaq tortg idif
DIFF  1.d-5  12.6          2.13d-1     1.8   1.d0  1.d0    0
: species diffusion coef [cm^2/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*(*θ*)-, 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)
02  (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 [ISYStem]

Initialization Data Keyword: **ISYStem**

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: ISYStem ISAT ISOTHRM IREAD PHIR POR0 SAT PORM SATM LAMBDA TOLPOR

ISYStem 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

PHIR Initial reacting volume fraction.

POR0 Initial porosity if constant. Not used in coupled mode.

SAT Liquie phase saturation. Not used in coupled mode.

PORM Matrix porosity. Not used in coupled mode or for single continuum simulations.

SATM Matrix liquid saturation. Not used in coupled mode or for single continuum simulations.

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

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  phir  por0  sat  porm  lambda satm  tolpor
ISYStem  0     1          0     1.    .1   0.5   0     1.      0   1.e-3
```

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

Comments(s):

In coupled mode porosity and saturations are specified by METRA.

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/cm^2/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 `nkmx` 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.
= 3 Use maximum change in concentration (**DELCMX**) 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  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 $T(X) = A + (B-A) EXP[-((X-X0)/C)^2] + (D-A) * X / XLEN$
= 3 T(X,T) = A + ½(B-A) (ERF[(X+C-X0)/(2SQRT(DT))] - ERF[(X-C-X0)/(2SQRT(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. **= -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 > Residual or TOLC $\geq$ max $|C_l^{k+1} - C_l^k|$.

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 [m^3].

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  rpmf(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.
 /
:       igrid    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

PhiK
: i1  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
:  i1  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    i1    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   dsmx  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: $CO_{2(g)}$ and $O_{2(g)}$; 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
  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  sothrm  iread  phir  por0   sat  porm  satm  lambda  toldelt  tolpor
ISYS  0      1       0     1   0.101   0     0     0     0     1.e-3   1.e-3
:
:
:     d0[cm^2/s]  delhaq[kJ/mol]  dgas[cm^2/s]  dgexp  tortaq  tortg  idif
DIFF  1.d-5       12.6            2.13d-1        1.8   1.d0    1.d0   0
:
:
: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+
mghco3+
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
:                               matrix     fracture
: 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 EXPLANATION OF OUTPUT RESULTS

Although most of the output is self-explanatory, some of the more important output variables requiring further explanation or clarification are described in this section.

4.1 Screen Display

During a run, information is displayed on the screen that shows the progress of the run and can aid the user in determining whether or not the run is progressing satisfactorily. The initial display gives the program (MULTIFLO, METRA, or GEM) the revision number and date and a copyright notice. Running METRA with the input file `1d.dat` gives the screen output:

```
--> open input file 1d.dat

            CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
                    SOUTHWEST RESEARCH INSTITUTE
   ________________________________________________________________

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

                     Prepared for the U.S. NRC

                            Version 2.0

                            August 2003

                  MASS AND ENERGY TRANSPORT MODEL

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

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) itrs...>
    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

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

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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 in 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 (`mcyc`), 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:

```
 mcyc 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
.............................................................................
 mcyc 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
.............................................................................
```

4.1.3 MULTIFLO Screen Display

Running MULTIFLO gives the screen display

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

```
   _/      _/  _/  _/  _/     _/_/_/_/_/  _/  _/_/_/_/_/  _/          _/  _/
  _/_/_/._/  _/  _/  _/         _/      _/  _/          _/        _/      _/
 _/  _/  _/  _/  _/  _/        _/      _/  _/_/        _/        _/      _/
_/  _/  _/   _/_/_/  _/_/_/   _/      _/  _/          _/_/_/_/    _/  _/
```

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```
--> Initialization METRA
--> open input file multi.dat
--> read initial data from file init.int
--> Initialization GEM
--> call readat icode = 3
```

This output indicates successful initialization by METRA and GEM. The next set of lines shows the storage requirements for METRA and GEM:

```
==================================================================
 Total Work Space Required for [aa] in  MULTIFLO =         154462
                      Assigned =        10000000
==================================================================
```

The database is read next followed by distribution of species calculations at each node and for the boundary conditions:

```
--> 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

--> 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)  itrs...>
   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
 mcyc kcyc iter iconv ifor     time    target   delt [y]  maspec ndts   itrtot
   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        mcyc
 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.   [1,g]         vl         vg [m/y]      cfl     cfg        mcyc
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.   [1,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 itrtot
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:

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

for *i*th component,

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

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 [°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

$$V_B = DX * DY * DZ, \tag{4-3}$$

for Cartesian geometry,

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

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

$$X_g^a = (P-P_v)/P, \tag{4-5}$$

where

$$P_v = \text{saturation pressure of water.} \tag{4-6}$$

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

$$T_{x_i} = \frac{2\kappa_i\kappa_{i-1}\Delta y_j\Delta z_\kappa}{\Delta X_i\kappa_{i-1} + \Delta X_{i-1}\kappa_i} \tag{4-7}$$

$$T_{y_i} = \frac{2\kappa_j\kappa_{j-1}\Delta x_i\Delta z_\kappa}{\Delta y_j\kappa_{j-1} + \Delta y_{j-1}\kappa_j} \tag{4-8}$$

$$T_{z_\kappa} = \frac{2\kappa_\kappa\kappa_{\kappa-1}\Delta x_i\Delta y_j}{\Delta z_\kappa\kappa_{\kappa-1} + \Delta z_{\kappa-1}\kappa_\kappa} \tag{4-9}$$

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

$$T_{x_i} = \frac{2\pi\,\kappa_i\kappa_{i-1}\Delta y_j\Delta z_\kappa}{\kappa_{i-1}\ln\dfrac{r_i}{r_{i-1/2}} + \kappa_i\ln\dfrac{r_{i-1/2}}{r_{i-1}}}, \tag{4-10}$$

$$T_{z_\kappa} = \frac{2\kappa_\kappa\kappa_{\kappa-1}\Delta x_i\Delta y_j}{\Delta z_\kappa\kappa_{\kappa-1} + \Delta z_{\kappa-1}\kappa_\kappa}. \tag{4-11}$$

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 (angle/2π) if the system is not a full 360°.

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

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

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

4.2.1.4 Binary-Diffusion Transmissibility

In the presence of vapor-air binary diffusion, the constant coefficients corresponding to these transmissibilities (T_{x_1}, T_y, T_z) are calculated from Eq. (4-13)

$$T_{x_i} = \frac{\omega\sqrt{\phi_i\tau_i\phi_{i-1}\tau_{i-1}}D^0_{va}\Delta y_j\Delta z_\kappa}{RT^\theta_0(\Delta x_i + \Delta x_{i-1})} \tag{4-13}$$

and similarly in y- and z-directions, where

ω — enhancement factor
τ — tortuosity factor
ϕ — porosity
D^0_{va} — binary diffusion coefficient [m²/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-H_2O, 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 H_2O, air, and energy unaccounted for in the solution at the end of a time step. Err-H_2O is computed as follows:

$$\text{Err-}H_2O = M_{H_2O}(t + \Delta t) - M_{H_2O}(t) - M_{H_2O} \text{ mass injected} \qquad (4\text{-}14)$$

`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,

$$\max_{n} \left| \Delta p_n^{\kappa}, \Delta p_{an}^{\kappa} \Delta s_n^{\kappa}, \Delta T_n^{\kappa} \right| < [tolp, tolpa, tols, tolt], \qquad (4\text{-}15)$$

where κ is the Newtonian iteration number, n refers to the node, and Δp_n^{κ}, Δp_{an}^{κ}, Δs_n^{κ}, and ΔT_n^{κ} represent the solution vectors. The parameters *tolp*, *tolpa*, *tols*, and *tolt* 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,

$$\max_{n} |R_{in}^{\kappa}| < [tolm, tola, tole] \qquad (4\text{-}16)$$

where R_{in}^{κ} 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*, *tola*, 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-H₂O`, 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_20, air, and energy are printed as $H_2$0BAL, AIRBAL, and ENRGBAL. H_2OINC, AIRINC, and ENRGINC 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-H₂O`, 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 is one spatial plot file for field variables and one for each component of 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/m^2/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).

4.3 GEM Output

The output file for GEM is called `fn.out`. 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 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 Table 4-4. Concentration histories for nodes specified by BRKP keyword are written to the file `fabrk.xyp`.

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_vel.xyp`	[xyz], vgx, vlx, vgy, vly, vgz, vlz
`jobname_flx.xyp`	[xyz], fgx, flx
`jobname_fly.xyp`	[xyz], fgy, fly
`jobname_flz.xyp`	[xyz], 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
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 GEM Plot Files Containing Spatial Profile Data at Times Specified on the TIME Keyword

File Name	Description
`maspltaq[n].xyp`	Aqueous concentrations
`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

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.

```
         ../multiflo
              |
      ---------------
      |             |
   metra           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
```

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   (Nxmx = 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.

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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

$$s_l^{\text{eff}} = \left[1 + \left(\alpha \, | P_c | \right)^m\right]^{-\lambda}, \qquad \text{(A–1)}$$

where P_c represents the capillary pressure [Pa], and s_l^{eff} is defined by

$$s_l^{\text{eff}} = \frac{s_l - s_l^r}{s_l^0 - s_l^r}, \qquad \text{(A–2)}$$

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

$$\lambda = 1 - \frac{1}{m}, \quad m = \frac{1}{1 - \lambda}. \qquad \text{(A–3)}$$

Relative permeability for the liquid phase is given by the expression

$$\kappa_{rl} = \sqrt{s_l^{\text{eff}}} \left\{1 - \left[1 - \left(s_l^{\text{eff}}\right)^{1/\lambda}\right]^{\lambda}\right\}^2, \qquad \text{(A–4)}$$

and for the gas phase by

$$\kappa_{rg} = 1 - \kappa_{rl}. \qquad \text{(A–5)}$$

A.1.2 Brooks-Corey Functions

The Brooks-Corey functions for relative permeability are defined by

$$\kappa_{rl} = s_*^4,\ \kappa_{rg} = \left(1 - s_*^2\right)\left(1 - s_*\right)^2,\ s_* = \frac{s_l - s_l^r}{1 - s_l^r - s_g^r}. \qquad \text{(A–6)}$$

Capillary pressure is not incorporated in the Brooks-Corey functions.

A.1.3 Linear

The linear relation is defined by

$$\kappa_{rl} = s_*,\ \kappa_{rg} = 1 - \kappa_{rl},\ s_* = \frac{s_l - s_l^r}{1 - s_l^r}. \qquad \text{(A–7)}$$

A.2 KELVIN'S EQUATIONS FOR VAPOR PRESSURE LOWERING

Vapor pressure lowering resulting from capillary suction is described by Kelvin's equation given by

$$P_v = P_{\text{sat}}(T)\, e^{-Pc/n_l RT}, \qquad \text{(A–8)}$$

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)

$$\text{CK} = \text{CKDRY} + \sqrt{s_l}\left(\text{CKSAT} - \text{CKDRY}\right), \qquad \text{(A–9)}$$

where CKDRY and CKSAT are dry and fully saturated rock thermal conductivities.

A.4 VAPOR-AIR DIFFUSION EQUATION

The conservation equation for the H$_2$0 component (w) is given by

$$\frac{\partial}{\partial t}\left[\phi\left(s_l n_l X_w^l + s_g n_g X_w^g\right)\right] + \nabla \cdot \left(q_l n_l X_w^l + q_g n_g X_w^g - D_g^{\text{eff}} n_g \nabla X_w^g\right) = Q_w, \tag{A–10}$$

and for the air component (a) by

$$\frac{\partial}{\partial t}\left[\phi\left(s_l n_l X_a^l + s_g n_g X_a^g\right)\right] + \nabla \cdot \left(q_l n_l X_a^l + q_g n_g X_a^g - D_g^{\text{eff}} n_g \nabla X_a^g\right) = Q_a, \tag{A–11}$$

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

$$q_l = -\frac{kk_l}{\mu_l}\nabla\left(P_l - \rho_l\, gz\right), \tag{A–12}$$

and

$$q_g = -\frac{kk_g}{\mu_g}\nabla\left(P_g - \rho_g\, gz\right), \tag{A–13}$$

where k 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

$$X_w^l + X_a^l = 1, \quad X_w^g + X_a^g = 1. \tag{A–14}$$

Diffusion of water in the aqueous phase is neglected. The liquid and gas pressures are related through the capillary pressure:

$$P_l = P_g - P_c, \tag{A–15}$$

The effective binary gas diffusion coefficient is defined in terms of temperature, pressure, and material properties by

$$D_g^{\text{eff}} = \omega\tau\phi s_g D_g^0 \frac{P_0}{P}\left[\frac{T+T_0}{T_0}\right]^\theta, \tag{A–16}$$

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:

$$\frac{\partial}{\partial t}\left[\phi\ (s_l n_l + s_g n_g)\right] + \nabla \cdot (q_l n_l + q_g n_g) = Q_w + Q_a. \tag{A–17}$$

A.5 ENERGY BALANCE EQUATION

The energy balance equation, assuming thermodynamic equilibrium between rock and fluid, is given by

$$\begin{aligned}\frac{\partial}{\partial t}\left[\phi\left(s_l n_l U_l + s_g n_g U_g\right)\right] + \nabla \cdot \left(q_l n_l H_l + q_g n_g H_g\right) \\ + \frac{\partial}{\partial t}\left[\left(1-\phi\right)C_p^{\text{rock}}\rho_{\text{rock}}T\right] - \nabla \cdot \kappa\nabla T = Q_e.\end{aligned} \tag{A–18}$$

where T denotes the temperature, U_π the total internal energy, and H_π the total enthalpy of the πth fluid phase, C_p^{rock} the heat capacity, κ the thermal conductivity, and Q_e 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 $2\,\delta$ and fracture-matrix interfacial area per bulk volume A_{fm} follows. Depending on the 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

$$V_m = \left(1 - \epsilon_f\right) V(\delta) \tag{A–19}$$

The interfacial surface area per bulk volume is computed from the relation

$$A_{fm} = \eta\, a_{fm}, \tag{A–20}$$

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

$$2\delta = l \frac{\epsilon_f}{1 - \epsilon_f}, \tag{A–21}$$

and the interfacial area per bulk volume

$$A_{fm} = \frac{2\left(1 - \epsilon_f\right)}{l}, \tag{A–22}$$

where $l = l_x = l_y = l_z$ represents the matrix block size.

Two-dimensional Geometry. In a two-dimensional system

$$V = \left(l_x + 2\delta\right)\left(l_y + 2\delta\right) \qquad \text{(A–23)}$$

and

$$V_m = l_x l_y. \qquad \text{(A–24)}$$

It follows that δ satisfies the quadratic equation

$$\delta^2 + \frac{1}{2}\left(l_x + l_y\right)\delta - \frac{\epsilon_f l_x l_y}{4\left(1 - \epsilon_f\right)} = 0. \qquad \text{(A–25)}$$

Solving this equation explicitly for 2δ yields the relation

$$2\delta = \frac{1}{2}\left\{\sqrt{\left(l_x + l_y\right)^2 + 4\frac{\epsilon_f l_x l_y}{1 - \epsilon_f}} - \left(l_x + l_y\right)\right\}. \qquad \text{(A–26)}$$

Three-dimensional Geometry. In a three-dimensional system

$$V = \left(l_x + 2\delta\right)\left(l_y + 2\delta\right)\left(l_z + 2\delta\right) \qquad \text{(A–27)}$$

and

$$V_m = l_x l_y l_z. \qquad \text{(A–28)}$$

The aperture satisfies the cubic equation

$$\delta^3 + b\delta^2 + c\delta + d = 0, \qquad \text{(A–29)}$$

where

$$b = l_x + l_y + l_z, \tag{A–30}$$

$$c = l_x l_y + l_y l_z + l_z l_x, \tag{A–31}$$

$$d = -\frac{\epsilon_f}{1 - \epsilon_f} l_x l_y l_z. \tag{A–32}$$

This equation has the explicit solution

$$\delta = \alpha + \beta - \frac{b}{3}, \tag{A–33}$$

where

$$\alpha = \left(\frac{u_2 + u_3}{2} \right)^{1/3} \tag{A–34}$$

$$\beta = \left(\frac{u_2 - u_3}{2} \right)^{1/3} \tag{A–35}$$

and

$$u_2 = -\left[d - \frac{1}{3}\, bc + \frac{2}{27}\, b^3 \right], \tag{A–36}$$

$$u_3 = \left[u_2^2 + \frac{4}{27}\left(c - \frac{b^2}{3}\right)^3\right]^{1/2}. \qquad \text{(A–37)}$$

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*:

$$\eta = \frac{V_m}{l_x l_y l_z} \qquad \text{(A–38)}$$

The number density η/V giving the number of matrix blocks per bulk volume is equal to

$$\frac{\eta}{V} = \frac{1 - \epsilon_f}{l_x l_y l_z} \qquad \text{(A–39)}$$

The interfacial area per matrix block is equal to

$$a_{fm} = 2\left(l_x l_y + l_y l_z + l_z l_x\right) \qquad \text{(A–40)}$$

Hence in three-dimensional the interfacial area per bulk volume is equal to

$$\begin{aligned} A_{fm}^{3D} &= \frac{\eta}{V} a_{fm}, \\ &= \left(1 - \epsilon_f\right) \frac{2\left(l_x l_y + l_y l_z + l_z l_x\right)}{l_x l_y l_z}, \\ &= 2\left(1 - \epsilon_f\right)\left[\frac{1}{l_x} + \frac{1}{l_y} + \frac{1}{l_z}\right]. \end{aligned} \qquad \text{(A–41)}$$

In two-dimensional:

$$A_{fm}^{2D} = 2(1 - \epsilon_f)\left[\frac{1}{l_x} + \frac{1}{l_y}\right], \tag{A–42}$$

and in one-dimensional:

$$A_{fm}^{1D} = 2(1 - \epsilon_f)\,\frac{1}{l}. \tag{A–43}$$

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

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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

$$\sum_{j=1}^{N_c} \nu^{l}_{ji} A_j \rightleftharpoons A^{l}_i, \qquad \left(i = 1,\dots,N_l\right), \qquad \text{(B–1)}$$

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^{l}_i. gaseous species A^{g}_i.

$$\sum_{i=1}^{N_c} \nu^{g}_{ji} A_j \rightleftharpoons A^{g}_i, \qquad \left(i = 1,\dots,N_g\right), \qquad \text{(B–2)}$$

and minerals M_m

$$\sum_{i=1}^{N_c} \nu_{jm} A_j \rightleftharpoons M_m, \qquad \left(i = 1,\dots,N_m\right), \qquad \text{(B–3)}$$

assumed to occur in numbers N_l, N_g, and N_m, respectively. The matrices ν^{l}_{ji}, ν^{g}_{ji}, and ν_{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

$$z_\kappa A_j^{z_j+} + z_j X_{z_\kappa} A_\kappa^{z_\kappa+} \rightleftharpoons z_j A_\kappa^{z_\kappa+} + z_\kappa X_{z_j} A_j^{z_j+}, \tag{B–4}$$

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 [$H_2O_{(l)}$] 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)

$$\frac{\partial}{\partial t}\left(\phi\psi_j + \overline{C}_y\right) + \nabla\cdot\Omega_j = -\sum_{m=1}^{N_m} \nu_{jm} I_m, \tag{B–5}$$

where $\overline{C}_j$ denotes the adsorbed concentration of the *j*th primary species, and the generalized concentration Ψ_j and flux Ω_j are defined by

$$\Psi_j = s_l \Psi_j^l + s_g \Psi_j^g, \tag{B–6}$$

and

$$\Omega_j = \Omega_j^l + \Omega_j^g, \tag{B–7}$$

with

$$\psi_j^\pi = \delta_{\pi l} C_j^\pi + \sum_{i=1}^{N_\pi} \nu_{ji}^\pi C_i^\pi \tag{B–8}$$

and

$$\Omega_j^\pi = \delta_{\pi l} J_j^\pi + \sum_{i=1}^{N_\pi} \nu_{ji}^\pi J_i^\pi, \tag{B–9}$$

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

$$\frac{\partial \phi_m}{\partial t} = \overline{V_m}\, I_m, \tag{B–10}$$

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 ith species in the πth phase, ϕ_m and $\overline{V_m}$ denote the volume fraction and molar volume, respectively, of the mth mineral. The liquid flux J_i^l appearing in these equations is defined by

$$J_i^l = -\varphi \tau s_l D_l \nabla C_i^l + q_l C_i^l \tag{B–11}$$

and the gas flux J_i^g by the equation

$$J_i^g = -\varphi \tau s_g D_g \nabla C_i^g + q_g C_i^g, \tag{B–12}$$

where D_π denotes the diffusion coefficient in phase π and q_π the velocity of phase π defined by Darcy's law as:

$$q_\pi = -\frac{\mathbf{k}\ \mathbf{k}_{r\pi}}{\mu_\pi} \nabla \left(P_\pi - \rho_\pi g z\right), \tag{B–13}$$

where k refers to the saturated permeability of the porous medium, $\mathrm{k}_{r\pi}$ 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 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

$$\Omega_j^\pi = \left(-\varphi\,\tau\,\boldsymbol{s}_\pi\,\boldsymbol{D}_\pi + \boldsymbol{q}_\pi\right)\psi_j^\pi, \tag{B–14}$$

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 jth 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

$$C_i^l = \rho_l^{\alpha-1}\left(\gamma_i^l\right)^{-1} K_i^l \prod_{j=1}^{N_0}\left(\gamma_j^l C_j^l\right)^{\nu_{ji}^l}, \tag{B–15}$$

where γ_i^l denotes the activity coefficient, K_i^l the equilibrium constant, and the quantity α providing a density correction from molality to molarity units, is defined by

$$\alpha = \rho_l^{\sum_{ji}\nu_{ji}^l}, \tag{B–16}$$

The concentrations of gaseous species are given by

$$c_i^g = \frac{K_i^g}{RT} \prod_{j=1}^{N_0} \left(\gamma_j^l c_j^l\right)^{\nu_{ji}^g} \tag{B–17}$$

The exchange isotherm $\overline{C_\kappa}$, 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,

$$K_{j\kappa} = \left[\frac{c_\kappa^l}{\overline{C_\kappa}}\right]^{z_j} \left[\frac{\overline{C_j}}{c_j^l}\right]^{z_\kappa}, \tag{B–18}$$

consistent with Eq. (B–4), where the quantities $K_{j\kappa}$ represent selectivity coefficients. Combining this relation with the site conservation equation

$$\omega = (1 - \phi)\,\rho_{\text{solid}}\, Q = \sum z_j \overline{C_j}, \tag{B–19}$$

where Q denotes the cation exchange capacity, yields a single nonlinear equation for the *j*th sorption isotherm $\overline{C_j}$

$$\omega = z_j \overline{C_j} + \sum_{\kappa \neq 1} c_\kappa^l K_{j\kappa}^{1/z_\kappa} \left[\frac{\overline{C_j}}{c_j^l}\right]^{z_j/z_\kappa} \tag{B–20}$$

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

$$\log K(T) = \frac{a_{-2}}{T^2} + \frac{a_{-1}}{T} + a_0 \ln T + a_1 + a_2 T, \tag{B–21}$$

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

$$A_m = -RT \ln K_m Q_m, \tag{B–22}$$

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

$$Q_m = \prod_{j=1}^{N_c} \left(\gamma_j^l C_j^l\right)^{\nu_{jm}}, \tag{B–23}$$

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

$$I_m = \begin{cases} \hat{I}_m, & \phi_m > 0 \text{ or } A_m < 0, \\ 0, & \text{otherwise} \end{cases} \tag{B–24}$$

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

$$\hat{I}_m = - s_m \left(\sum_l P_{ml}\, \kappa_{ml}\right) \left[1 - \left(K_m Q_m\right)^{\sigma_m}\right], \tag{B–25}$$

where the prefactor P_{ml} is defined as

$$P_{ml} = \prod_{j=1}^{N_c} a_j^{\alpha_{jl}^m} \prod_{i=1}^{N_{cx}} a_i^{\alpha_{il}^m}, \tag{B–26}$$

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 Tempkin's constant a_i represents the activity of the ith species, and α_{jl}^m, α_{il}^m are constants. With this form of the rate, the effective kinetic rate constant κ_m may be pH-dependent with the form

$$\kappa_m = \kappa_m^a a_{H+}^{\beta a} + \kappa_m^b a_{H+}^{\beta b} + \kappa_m^0, \tag{B–27}$$

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

$$\hat{I}_m = -s_m \sum_l P_{ml}\, \kappa_{ml} \left[\frac{1 - \left(K_m Q_m\right)^{\sigma_m}}{1 + \dfrac{P_{ml}\, \kappa_{ml}}{r_{\lim}} \left(K_m Q_m\right)^{\sigma_m}}\right] \tag{B–28}$$

with transport-limited rate $r_{\lim}$. For $Q_m \rightarrow \infty$,

$$\hat{I}_m \rightarrow N_m^p\, r_{\lim} \tag{B–29}$$

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

$$s_m^V = \phi \rho_f s_m^M, \tag{B–30}$$

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), ρ_f 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

$$s_m^V = \frac{6}{b_m} \phi_m, \tag{B–31}$$

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:

$$\kappa_m(T) = \kappa_m^0 \frac{T}{T_0} \exp\left[-\left(\frac{1}{T} - \frac{1}{T_0}\right)\frac{\Delta H_m^\dagger}{R}\right], \tag{B–32}$$

where k_m^0 denotes the rate constant at reference temperature T_0 and $\Delta H_m^\dagger$ denotes the enthalpy of activation.

For kinetic homogeneous aqueous reactions a rate law of the form

$$I_j = -\left(\sum_l P_{jl}\kappa_{jl}\right)\left[1 - K_j Q_j\right], \tag{B–33}$$

and an analogous transport-limited form

$$I_j = -\sum_l P_{jl}\,\kappa_{jl}\left[\frac{1 - K_j Q_j}{1 + \dfrac{P_{jl}\kappa_{jl}}{r_{\lim}}K_j Q_j}\right], \tag{B–34}$$

is used. The ion activity product Q_j is defined as

$$Q_j = \left(a_j^l\right)^{-1}\prod_{j'=1}^{N_c}\left(\gamma_{j'}^l C_{j'}^l\right)^{\nu_{j'l_i}}, \tag{B–35}$$

where a_j^l 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

$$\phi = 1 - \sum_{m=1}^{N_m}\phi_m. \tag{B-36}$$

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

$$\kappa = \kappa_0\left(\frac{\phi}{\phi_0}\right)^n, \tag{B–37}$$

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

$$\tau = \tau_0 \left(\frac{\varphi}{\varphi_0} \right)^n , \tag{B–38}$$

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

$$s_m = s_m^0 \left(\frac{\phi \, \phi_m}{\phi_0 \, \phi_m^0} \right)^{2/3} , \tag{B–39}$$

for primary minerals $\left(\varphi_m^0 > 0\right)$, and

$$s_m = s_m^0 \left(\frac{\phi}{\phi_0} \right)^{2/3} , \tag{B–40}$$

for secondary minerals $\left(\varphi_m^0 > 0\right)$. 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:

$$\phi_m(r, t + \Delta t) = \phi_{m'}(r, t) + \Delta t\, \overline{V_m}\, I_m(r, t), \qquad \text{(B–41)}$$

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)*

$$F(t') = \left(1 - \frac{t' - t}{\Delta t}\right) F(t) + \left(\frac{t' - t}{\Delta T}\right) F(t + \Delta t), \qquad \text{(B–42)}$$

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 formulation 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 $\tilde{\psi}^l_j\left(r,t+\Delta t\right)$ and $\tilde{\psi}^g_j\left(r,t+\Delta t\right)$ where the tilde (~) indicates nonreactive transport and *l* (*g*) refers to liquid (gas). The nonreactive transport equations for aqueous and gaseous species read:

$$\frac{\partial}{\partial t}\left(\varphi\, s_\pi\, \tilde{\psi}^\pi_j\right) + \nabla \cdot \tilde{\Omega}^\pi_j = \mathbf{0}\,, \tag{B–43}$$

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

$$\frac{\partial}{\partial t}\left[\phi\left(s_l \psi_j^l + s_g \psi_j^g\right)\right] = -\sum_m \nu_{jm} I_m \,, \qquad \text{(B–44)}$$

is solved, subject to the initial condition

$$\psi_j^\pi(\boldsymbol{r},\boldsymbol{t}) = \tilde{\psi}_j^\pi(\boldsymbol{r},\boldsymbol{t}+\Delta \boldsymbol{t}), (\pi = \boldsymbol{l},\boldsymbol{g}) \qquad \text{(B–45)}$$

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

$$\frac{\partial}{\partial \boldsymbol{t}}\left(\varphi\, \boldsymbol{s}_\pi\, \tilde{\psi}_j^\pi\right) + \nabla \cdot \tilde{\Omega}_j^\pi = 0 \,, \quad (\pi = \boldsymbol{l},\boldsymbol{g}) \qquad \text{(B–46)}$$

which is followed by the reactive step

$$\frac{\partial}{\partial t}\left[\varphi\left(s_l \hat{\psi}_j^l + s_g \hat{\psi}_j^g\right)\right] = -\sum_m \nu_{jm} I_m \,, \qquad \text{(B–47)}$$

subject to initial conditions

$$\hat{\psi}_j^{\pi}(\boldsymbol{r},\boldsymbol{t}) = \tilde{\psi}_j^{\pi}\left(\boldsymbol{r},\boldsymbol{t} + \frac{\Delta t}{2}\right), \quad (\pi = \boldsymbol{l},\boldsymbol{g}) \tag{B–48}$$

The final transport step uses this total concentration as an initial condition to obtain the desired concentration at time $\Delta t \,/\, 2$:

$$\frac{\partial}{\partial \boldsymbol{t}}\left(\varphi\, \boldsymbol{s}_{\pi}\, \psi_j^{\pi}\right) + \nabla \cdot \Omega_j^{\pi} = 0\,, \quad (\pi = \boldsymbol{l},\boldsymbol{g}) \tag{B–49}$$

$$\psi_j^{\pi}\left(\boldsymbol{r},\boldsymbol{t} + \frac{\Delta t}{2}\right) = \hat{\psi}_j^{\pi}\left(\boldsymbol{r},\boldsymbol{t} + \Delta t\right), \quad (\pi = \boldsymbol{l},\boldsymbol{g}) \tag{B–50}$$

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.

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