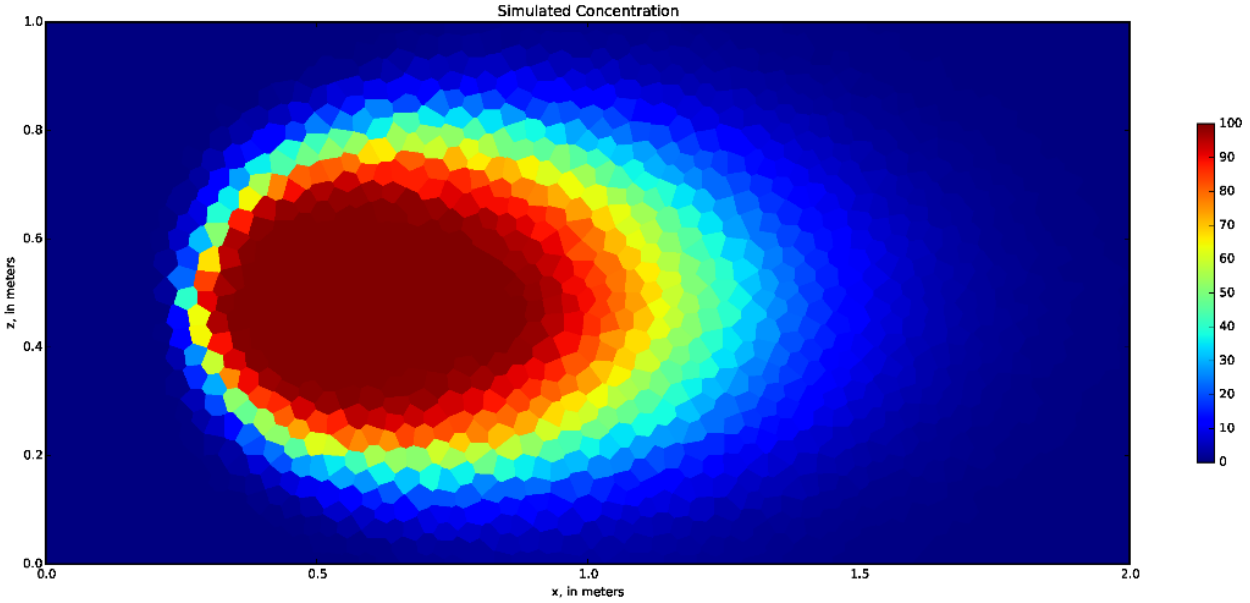
USG-TRANSPORT: TRANSPORT AND OTHER ENHANCEMENTS TO MODFLOW-USG

Version 2.5.0



Input Instructions Document

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Cover: The cover image depicts results from a simulation of transport in a uniform flow field using an unstructured mesh. Courtesy Christian D. Langevin.

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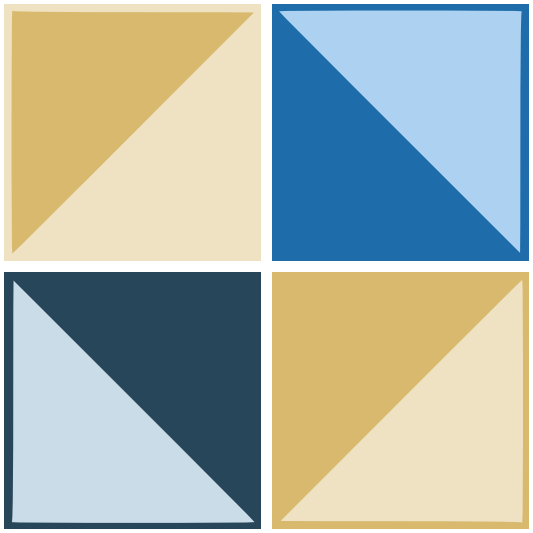

MODFLOW-USG-Transport

Sorab Panday

PREFACE

The computer model described in this report is ***MODFLOW-USG-Transport***, released by GSI Environmental. The code and documentation are currently available for downloading from the GSI Website https://www.gsienv.com/product/modflow-usg/. Newer versions or releases with revisions and updates will be made available for downloading from the same website. Alternatively, the user can register at the GSI Website for emails that make users aware of code updates.

MODFLOW-USG-Transport (or USG-T), includes advancements to the MODFLOW-USG software first released by the U.S. Geological Survey (USGS) in 2013. The primary functional capability that has been added in USG-T is simulation of three-dimensional chemical species transport. The transport module works seamlessly with the MODFLOW-USG groundwater flow model and is fully compatible with flow-fields generated by the Groundwater Flow (GWF) and Connected Linear Network (CLN) Processes of MODFLOW-USG.

Other updates to MODFLOW-USG flow routines are also published with USG-T which include, among other processes or convenient features, unsaturated zone flow and transport, turbulent formulations for CLN flow, and density dependent flow transport coupling.

Testing of the new USG-T routines indicated that the code yields reliable, mass conserved results for a wide variety of problems. The user, however, should be aware that the accuracy and efficiency of transport computations can be significantly affected by gridding and time-stepping considerations among other conceptual and numerical factors. A recorded webinar on transport fundamentals, specifically with USG-T, is available commercially from the GSI Environmental website at https://www.gsienv.com/webinars/webinar-3-simulation-of-solute-and-heat-transport-with-usg-transport-and-other-general-transport-simulation-fundamentals/.

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ACKNOWLEDGMENTS

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DISCLAIMER

The authors of this work and GSI Environmental make no warranties and disclaim liability for **all uses of the software and documentation**.

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ABSTRACT

This report presents the I/O documentation for MODFLOW-USG-Transport (USG-T). The input instructions for all USG-T modules are consolidated in this document.

USG-T includes advancements to the MODFLOW-USG software first released by the U.S. Geological Survey (USGS) in 2013. The major advancement to MODFLOW-USG is inclusion of capability to simulate solute and heat transport using the Block Centered Transport (BCT) process. USG-T also enhances the MODFLOW-USG flow capabilities which are documented here as well. The complete document for MODFLOW-USG and the input and output instructions are available from the USGS website (Panday et al., 2013) and should be used as a reference guide.

The BCT process has been developed using a Control Volume Finite Difference (CVFD) scheme that is fully compatible with and integrated into MODFLOW-USG (Panday et al., 2013), which was released by the U.S. Geological Survey, is a three-dimensional groundwater flow model that uses implicit Control Volume Finite Difference (CVFD) methods to solve for steady-state and/or transient flow on unstructured grids. MODFLOW-USG includes a Groundwater Flow (GWF) Process and a Connected Linear Network (CLN) flow process. The GWF Process solves for flow in a three-dimensional porous medium. The CLN flow process solves for flow through a network of 1-dimensional cells representing wells, rivers, or fracture networks, interacting with the GWF process. Transport is fully compatible with flow in the GWF domain and within the CLN domain and accommodates solute migration between the CLN domain and the GWF domain as part of the solution. The numerical schemes are selected to provide optimal solution speed and accuracy pertinent to most subsurface transport simulation objectives.

DESCRIPTION OF INPUT FILES

Input file formats and structures for USG-T are similar to those of the MODFLOW-USG flow packages, and options are available to enter data for structured finite-difference grids or for general unstructured grids. The unstructured grid input is highlighted by use of a blue font to delineate this information for convenience. Different color fonts (including blue) are used to note enhanced capabilities to the original MODFLOW packages, to draw attention to the additional capabilities. For the new USG_T packages, different color fonts are used to separate different capabilities. In the block-centered transport module inputs for instance, the various options are

kept separate with different color fonts so users can ignore capabilities they are not using (heat transport is in brown, PFAS air-water interface adsorption is in green in the BCT package input).

Input formats and structures for the MODFLOW-USG and USG-T packages follow those of MODFLOW-2005. The main difference when using an unstructured grid is that instead of using layer, row and column numbers to identify a cell, the cell numbers are identified directly. The option is also available within the flow packages, to allow for structured finite difference grid input, as used in MODFLOW-2005; therefore, any MODFLOW-2005 input file may be used with MODFLOW-USG after accommodation of solver input. MODFLOW-USG and USG-T inputs use the standard package formats provided with MODFLOW-2005, with addition of options, flags, or data to address the enhanced capabilities. Options and flags are also used to incorporate newer features that may require additional file handling, which allows updates to USG-T to be backward compatible with input files from previous versions of the code.

Note that the center of a cell is termed the node in this document and hence terms like “number of cells”, or “number of nodes” may have been used interchangeably.

BASIC (BAS) PACKAGE INPUT INSTRUCTIONS

The Basic Package reads several files: Name File, Discretization File, Basic Package file, Multiplier Array file, Zone Array file, Output Control Option file, the Time-Variant Specified-Head Option file, and the Parameter Value File. The Name File, Discretization File, and Basic Package File are required for all simulations. The other files are optional. The Name File, Basic Package file and Discretization File, are modified from MODFLOW-2005 for use with unstructured grid input.

Name File

The Name File contains the names of most of the input and output files used in a model simulation and controls whether or not parts of the model program are active. (“OPEN/CLOSE” files, described in the Input Instructions for Array Reading Utility Subroutines section, are not included in the Name File.) The Name File is read on unit 99. The Name File is constructed as follows.

FOR EACH SIMULATION

1. Ftype Nunit Fname [Fstatus]

The Name File contains one of the above lines (item 1) for each file. All variables are free format. The length of each line must be 299 characters or less. The lines can be in any order except for the line where Ftype (file type) is "LIST" as described below.

Comment lines are indicated by the # character in column one and can be located anywhere in the file. Any text characters can follow the # character. Comment lines have no effect on the simulation; their purpose is to allow users to provide documentation about a particular simulation. All comment lines are written in the listing file.

Explanation of Variables in the Name File:

Ftype—is the file type, which must be one of the following character values. Ftype may be entered in any combination of uppercase and lowercase. (For users of MODFLOW-2000, the GLOBAL file type is no longer supported in MODFLOW-2005 or MODFLOW-USG.) Also note that the HUF Package is not currently supported by MODFLOW-USG and that the UPW Package capability is included through a flag in the BCF6 or LPF packages. Further, the traditional MODFLOW solver packages are not supported because they only handle structured grids. Instead, the SMS Package presents several linearization and sparse matrix solver options for solution to the fully coupled groundwater and CLN flow equations.

BAS6 for the Basic Package

BCF6 for the Block-Centered Flow Package

BCT for the Block Centered Transport Package

CHD for the Time-Variant Specified-Head Option

CLN for the Connected Linear Network Process

DPF for the Dual Porosity Flow Package

DPT for the Dual Porosity Transport Package

DDF for the Density Dependent Flow Package

DIS for the Discretization File for a structured grid

DISU for the Discretization File for an unstructured grid

DRN for the Drain Package

ETS for the Segmented Evapotranspiration Package

EVS for the Evapotranspiration Time-Series Package

EVT for the Evapotranspiration Package

FHB for the transient Flow and Head Boundary Package

GAGE for the Gage Package

GHB for the General-Head Boundary Package

GNC for the Ghost Node Correction Package

HFB6 for the Hydraulic Flow Barrier Package

SYF for the specific yield file as required for an IHM simulation. ***See IHM integration with USG-T section and input instructions for details.***

LAK for the Lake Package

LIST for the Listing File—This type must be present and must be the first file in the Name File.

LPF for the Layer Property Flow package

MDT for the Matrix Diffusion Transport Package

MULT for the multiplier array file

OC for the Output Control Option

PCB for the Prescribed Concentration Package

PVAL for the Parameter Value File

RCH for the Recharge Package

RIV for the River Package

RTS for the Recharge Time-Series Package

STR for the Streamflow Package

SFR2 for the Streamflow Routing Package

SMS for the Sparse Matrix Solver Packages – Currently available SMS packages include:

- ***XMD*** for the χMD Solution Package of Ibaraki (2005)

- ***PCGU*** for the unstructured pre-conditioned conjugate gradient package of White and Hughes (2011)

WEL for the Well Package

ZONE for the zone array file

Note that the DIS and DISU files cannot be used together in the same simulation, similarly with the BCF6 and LPF files.

DATA(BINARY) for binary (unformatted) files, such as those used to save cell-by-cell budget data and binary (unformatted) head and drawdown data. Files of this type are rewound at the start of each parameter estimation iteration.

DATA for formatted (text) files, such as those used to save formatted head and drawdown and for input of data from files that are separate from the primary package input files. Files of this type are rewound at the start of each parameter-estimation iteration. The Debug file (if written) for an IHM simulation will be of this type. ***See IHM integration with USG-T section and input instructions for details.***

Nunit—is the Fortran unit number to be used when reading from or writing to the file. Any legal unit number on the computer being used can be specified except unit 99. Unit 99 is used for the Name File and for reading multi-valued variables using the OPEN/CLOSE option of the utility subroutines (see Input Instructions for Array Reading Utility Subroutines section). The unit number for each file must be unique.

Fname—is the name of the file, which is a character value. Pathnames may be specified as part of Fname.

Fstatus—is the optional file status, which applies only to file types Data and Data(Binary).

> **Fstatus** can be either OLD or REPLACE. “Old” indicates that the file should already exist. “Replace” indicates that if the file already exists, then it should be deleted before opening a new file. ***The default is to open the existing file if the file exists or create a new file if the file does not exist.***
>
> **Fstatus** can also be the keyword FLUSH. If this keyword is used, then the associated files are flushed from buffer onto the disk at every time step of simulation. This allows for user to debug an issue if a simulation fails.

NO-ARCHIVE—For an IHM simulation, NO-ARCHIVE is a keyword that applies to all file types. The NO-ARCHIVE keyword is not applicable to a non-IHM (groundwater only) simulation with USG-T and will be ignored if used. ***See IHM integration with USG-T section and input instructions for details.***

- For input or output files accessed by IHM, the following applies:
    - If the NO-ARCHIVE keyword is used (i.e., file is "Replaced"), then USG-T closes the file at the start of each stress period and pauses until IHM provides a message to continue. For input files, IHM overwrites (replaces) the file prior to beginning groundwater flow computations using USG-T. For output files, USG-T overwrites (replaces) the file such that the file contains no more than one stress period of output. For an IHM simulation, IHM will force all USG-T binary output files (heads, drawdowns, or cell-by-cell flows) that are accessed by IHM to use the NO-ARCHIVE keyword because IHM uses a customized process to create binary files that contain results for the entire simulation. At the end of an IHM simulation a "Replaced" file contains data for only the last stress period of a simulation.
    - If the NO-ARCHIVE keyword is not used (i.e., file is "Archived"), then USG-T keeps the file open during the entire simulation. For input files, IHM appends data to the file at the start of the next stress period and USG-T reads the appended data for groundwater flow computations of that stress period. If IHM fully populated the file at simulation startup, IHM ensures that the NO-ARCHIVE flag was not applied to the file to prevent the modification of the file during the simulation and to ensure that USG-T reads the correct stress-period information. At the end of an IHM simulation an "Archived" file contains data for all stress periods.
- For input or output files not accessed by IHM, the following applies:
    - If the NO-ARCHIVE keyword is used (i.e., file is "Replaced"), then USG-T closes the file at the start of each stress period. This option is unlikely to be used when a file is not accessed by IHM. For input files, USG-T will open and read the same data at the start of each stress period if the file contains temporally dependent data (like boundary conditions). For output files, USG-T will open and write data

for each stress period, leaving output for only the last stress period at the end of the simulation.

- If the NO-ARCHIVE keyword is not used (i.e., file is "Archived"), then USG-T keeps the file open during the entire simulation. For input files, USG-T reads temporally dependent input data defined for each stress period. For output files, USG-T appends to the file at each stress period. For a binary cell-by-cell flow output file that is not accessed by IHM because it is produced by an USG-T package that has not been integrated within IHM, the output data for all integration time-steps is appended to the file.
- For an input DATA file containing material parameters or grid parameters that do not change through a simulation, the NO-ARCHIVE keyword should not be used because it adds more input to the NAME file with no change to model results or efficiency performance. DATA files of this type are read once by USG-T at simulation startup whether or not the NO-ARCHIVE keyword is present.

Note that the "Archived" mode is the default mode of a groundwater only simulation with USG-T as the code reads and writes data for every stress period of a model simulation. Also, the NO-ARCHIVE mode should not be used with a USG-T simulation otherwise it will repeatedly read the same (first) stress-period information thinking that the information was replaced.

Basic (BAS6) Package File

The Basic (BAS6) Package file is specified with "BAS6" as the file type. Note that if the discretization file type is DISU then the simulation is for an ***UNSTRUCTURED*** grid. An unstructured grid may also be used with the DIS file type if the associated option is provided. The BAS package has additional options of indicating if head / drawdown / concentration output and input could be double precision binary files.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. Options (199 text characters)

If there are no options to specify, then a blank line must be included for Item 1.

Item 2 is read for layer 1 first; then for layer 2 and so forth. Note that there may be a different number of nodes specified for each layer (NDSLAY) for an unstructured grid.

If *UNSTRUCTURED* option is used then read item 2a.

2a. IBOUND(NDSLAY) – U1DINT

If not a cross section, a layer variable is read for each layer in the grid.

If a cross section, NLAY rows of NDSLAY values are read. (NLAY being the number of layers and NDSLAY being the number of cells within each layer)

Otherwise, if *UNSTRUCTURED* option is not used then read item 2b for structured input

2b. IBOUND(NCOL,NROW) or (NCOL,NLAY) -- U2DINT

If not a cross section, NROW rows of NCOL values are read.

If a cross section, NLAY rows of NCOL values are read.

3. HNOFLO (10-space field unless Item 1 contains 'FREE'.)

Item 4 is read for layer 1 first, then for layer 2, and so forth. Note that there may be different number of nodes per layer (NDSLAY) for an unstructured grid.

If *UNSTRUCTURED* option is used then read item 4a.

4a. STRT(NDSLAY) – U1DREL

If not a cross section, the starting-head is read for each layer in the grid where NDSLAY is the number of nodes in the layer.

Otherwise, if *UNSTRUCTURED* option is not used then read item 4b for structured input

4b. STRT(NCOL,NROW) or (NCOL,NLAY) -- U2DREL

If not a cross section, the starting head is read for each layer in the grid.

If a cross section, NLAY rows of NCOL values are read.

Explanation of Variables Read from the BAS Package File

Text—is a character variable that starts in column 2. The first two comment lines will become variable HEADNG, which is used as a printout title throughout the program. (If there are no

comment lines, then HEADNG will be blank.) HEADNG is limited to 80 columns, but subsequent Text lines can be up to 199 columns. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

Options—is a character variable that is scanned for words (separated by one or more spaces) that specify program options. Six options are currently recognized. Unrecognized words are ignored, and a word may be specified in either uppercase or lowercase. A blank line is acceptable and indicates no options.

PRINTFV indicates that the finite-volume connectivity information for a regular grid is printed in the output file after being internally generated by the code. This option also prints the IA and JA arrays for structured or unstructured grids after being modified by the code to include CLN and GNC Packages.

XSECTION indicates that the model is a 1-row cross section for which STRT and IBOUND should each be read as single two-dimensional variables with dimensions of NCOL and NLAY for a structured grid. For an unstructured grid, NLAY rows of NDSLAY values are read. Likewise, head and drawdown should be printed and saved in disk files as single two-dimensional variables.

CHTOCH indicates that flow between adjacent constant-head cells should be calculated.

PRINTTIME indicates that a printout of the simulation time is required at the end of the simulation.

FREE indicates that free format is used for input variables throughout the Basic Package and other packages as indicated in their input instructions. Be sure that all variables read using free format have a non-blank value and that a comma or at least one blank separates all adjacent values.

UNSTRUCTURED indicates that an unstructured grid is used for the simulations. If the DISU package is used for discretization, an unstructured grid is assumed and this option is not needed. This option directs USG-T to use unstructured grid input even if the DIS package is used for discretization.

CONVERGE indicates that convergence is forced and the model will continue running even if the model fails to converge any time step. This option is an addition to MODFLOW-2005 capabilities and is useful to prevent termination of parameter estimation simulations if some of the forward runs do not converge.

RICHARDS indicates that the Richards' Equation will be used for the simulation in all layers of the model. A Richards' Equation solution may also be invoked in the BCF / LPF package for each layer by setting the LAYCON / LAYTYP flag appropriately.

DPIN indicates that binary input files for heads or concentrations are in double precision format. The time variables within these files also should be double precision variables.

DPOUT indicates that binary files for heads or concentrations will be written in double precision format. The time variables within these files also will be written as double precision variables.

DPIO indicates that binary input and output files for heads or concentrations are in double precision format. The time variables within these files also will be double precision variables.

IHM iuno indicates that the simulation is for an integrated hydrologic model (IHM). The keyword "***IHM***" is followed by a number "***iuno***" which indicates if the IHM simulation debugging information is saved or not. ***If iuno = 0***, the debugging information is not saved. ***If iuno = positive number***, it represents the Fortran Unit number of the file on which the debugging information is written. Note that if iuno is positive, the same number should be used in the NAME file to open the IHM debugging file with filetype of DATA. If keyword "***IHM***" is missing, the USG-T code is executed without the IHM integration modules being invoked. ***See IHM integration with USG-T section and input instructions for details.***

SY-ALL indicates that an IHM simulation will replace the specific yield array (SY) for all convertible layers at each integration time step. The default of an IHM simulation, when SY-ALL is not used, is to replace SY for only layer 1. Note that the simulation NAME file should also open the specific yield file using the SYF keyword such that the specific yield is passed between IHM and USG-T. The Specific Yield (SYF) File section of this document provides input details for structured and unstructured grids with SY-ALL option being absent or present.

IBOUND—is the boundary variable. One value is read for every model cell. Usually, these values are read one layer at a time; however, when the XSECTION option is specified, a single two-dimensional variable for the cross section is read. Note that although IBOUND may be read as one or more two-dimensional variables, IBOUND is stored internally only as a one-dimensional variable for all nodes in the domain.

If IBOUND(J,I,K) < 0, cell J,I,K has a constant head.

If IBOUND(J,I,K) = 0, cell J,I,K is no flow.

If IBOUND(J,I,K) > 0, cell J,I,K is variable head.

HNOFLO—is the value of head to be assigned to all no-flow cells (IBOUND = 0). Because head at no-flow cells is unused in model calculations, this does not affect model results but serves to identify no-flow cells when head is printed. This value is used also as drawdown at no-flow cells if the drawdown option is used. Even if the user does not anticipate having no-flow cells, a value for HNOFLO must be entered.

STRT—is initial (starting) head—that is, head at the beginning of the simulation. STRT must be specified for all simulations, including steady-state simulations. One value is read for every model cell. Usually, these values are read a layer at a time. When the XSECTION option is specified, however, a single two-dimensional variable for the cross section is read. If the *UNSTRUCTURED* option is selected, then the number of nodes within a layer may not be the same for all layers and thus the STRT array may be of different sizes for the different layers. For simulations in which the first stress period is steady state, the values used for STRT generally do not affect the simulation [exceptions may occur if cells go dry and (or) rewet]. The execution time, however, will be less if STRT includes hydraulic heads that are close to the steady-state solution.

Multiplier Array (MULT) File

Input to define multiplier arrays is read from the file that is specified with "MULT" as the file type. Multiplier arrays can be used to calculate layer variables from parameter values.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. NML

2. MLTNAM [FUNCTION]

If Item 2 does not contain the optional FUNCTION keyword, read Item 3 (3a or 3b):

If UNSTRUCTURED option is used then read item 3a.

3a. RMLT(NDSLAY) – U1DREL

Otherwise, if UNSTRUCTURED option is not used then read item 3b for structured input

3b. [RMLT(NCOL,NROW)] - U2DREL

Otherwise, if Item 2 contains the optional FUNCTION keyword, read Item 4:

4. [MLTNAM1 [op1 MLTNAM2] [op2 MLTNAM3] [op3 MLTNAM4] ...]

Repeat items 2 through 4 for each of the NML multiplier arrays.

Explanation of Variables Read from the Multiplier File:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NML—is the number of multiplier arrays to be defined.

MLTNAM—is the name of a multiplier array. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case are equivalent. The name "NONE" is a reserved word and should not be used for a multiplier array.

FUNCTION—is an optional keyword, which indicates that the multiplier array will be constructed from other multiplier arrays that have already been defined. Construction is by arithmetic combinations of the multipliers; see the explanation below for variable op1, op2, op3 ....

RMLT—is a two-dimensional (one layer) multiplier array.

MLTNAM1, MLTNAM2, MLTNAM3, ...—are the names of multiplier arrays that have already been defined.

op1, op2, op3, ...—are arithmetic operators used to define a multiplier array based on other multiplier arrays. Each operator can be either "+", "-", "*", or "/". Operations are applied from left to right to each array element. The operators must be separated from the multiplier array names by at least one space.

The following example input illustrates the use of the FUNCTION keyword to construct a multiplier array from other multiplier arrays. In this example, three multiplier arrays are defined, and accordingly the first line of the file contains "3". The first two arrays (named M1 and M2) are read using the U2DREL utility array reader (item 3), and the third array (named M3) is defined as the sum of M1 and M2. In this example, a model layer has 5 rows and 4 columns.

```
3
M1
INTERNAL 1.0 (4F6.0) 0
1.0 1.1 1.2 1.3
1.0 1.1 1.2 1.3
2.0 2.2 2.4 2.6
2.0 2.2 2.4 2.6
1.0 1.1 1.2 1.3
M2
INTERNAL 1.0 (4F6.0) 0
5.0 5.1 5.2 5.3
5.0 5.1 5.2 5.3
6.0 6.1 6.2 6.3
6.0 6.1 6.2 6.3
5.0 5.1 5.2 5.3
M3 FUNCTION
M1 + M2
```

The resulting values for multiplier M3 are:

```
6.0 6.2 6.4 6.6
6.0 6.2 6.4 6.6
8.0 8.3 8.6 8.9
```

```
8.0 8.3 8.6 8.9
6.0 6.2 6.4 6.6
```

Zone Array (ZONE) File

Input to define zone arrays is read from the file that is specified with "ZONE" as the file type. Zone arrays can be used to specify the cells in a layer variable that are associated with a parameter.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. NZN

2. ZONNAM

3. IZON(NCOL,NROW) - U2DINT

Items 2-3 are repeated for each of the NZN zone arrays.

Explanation of Variables Read from the Zone File:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NZN—is the number of zone arrays to be defined.

ZONNAM—is the name of a zone array. This name can consist of 1 to 10 characters and is not case sensitive; that is, any combination of the same characters with different case are equivalent. The name "ALL" is a reserved word and should not be used for a zone array.

IZON—is a two-dimensional (one layer) zone array.

Time-Variant Specified-Head (CHD) Option

Input to the Time-Variant Specified-Head (CHD) Option is read from the file that has file type "CHD" in the Name File. Optional variables are shown in brackets. All variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format.

Once a cell is made constant head, the cell stays constant head throughout the remainder of the simulation. For example, if a cell is listed in the CHD file as constant head in stress period 1 and not listed in stress period 2, then the cell continues to be constant head in stress period 2 and throughout the remainder of the stress periods. The head is adjusted only in the stress periods in which a cell is listed. For the stress periods in which a constant-head cell is not listed, the head stays at the value that it had at the end of the previous stress period.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—“#” must be in column 1. Item 0 can be repeated multiple times.

1. [PARAMETER NPCHD MXL]

This optional item must start with the word “PARAMETER”.

2. MXACTC [Option]

3. [PARNAM PARTYP Parval NLST]

If UNSTRUCTURED option is used then read item 4a.

4a. [Node Shdfact Ehdfact [xyz]]

Otherwise, if UNSTRUCTURED option is not used then read item 4b for structured input

4b. [Layer Row Column Shdfact Ehdfact [xyz]]

Repeat Items 3 and 4 NPCHD times. Items 3 and 4 are not read if NPCHD is negative or 0.

NLST repetitions of Item 4 are required; they are read by subroutine ULSTRD. (SFAC of the ULSTRD utility subroutine applies to Shdfact and Ehdfact).

FOR EACH STRESS PERIOD

5. ITMP NP

If UNSTRUCTURED option is used then read item 6a.

6a. Node Shdfact Ehdfact [xyz]

Otherwise, if UNSTRUCTURED option is not used then read item 6b for structured input

6b. Layer Row Column Shdfact Ehdfact [xyz]

ITMP repetitions of Item 6 are read by subroutine ULSTRD if ITMP > 0. (SFAC of the ULSTRD utility

subroutine applies to Shead and Ehead.) Item 6 is not read if ITMP is negative or 0.

7. [Pname]

(Item 7 is repeated NP times. Item 7 is not read if NP is negative or 0.)

Explanation of Variables Read by the CHD Option:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPCHD—is the number of constant-head boundary parameters.

MXL—is the maximum number of constant-head-boundary cells that will be defined using parameters.

MXACTC—is the maximum number of constant-head boundary cells in use during any stress period, including those that are defined using parameters.

Option—is an optional list of character values.

"AUXILIARY abc" or "AUX abc"—defines an auxiliary variable, named "abc", which will be read for each constant-head boundary as part of Items 4 and 6. Up to 20 variables can be specified, each of which must be preceded by "AUXILIARY" or "AUX." These variables will not be used by the Ground-Water Flow Process, but they will be available for use by other processes. The auxiliary variable values will be read after the Ehead variable.

"NOPRINT"—specifies that lists of constant-head cells will not be written to the Listing File.

PARNAM—is the name of a parameter. This name can consist of 1 to 10 characters and is not case sensitive; that is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter to be defined. For the CHD Package, the only allowed parameter type is CHD, which defines values of the start and end head at the boundary.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NLST—is the number of constant-head cells that are included in the parameter.

Layer—is the layer number of the constant-head boundary.

Row—is the row number of the constant-head boundary.

Column—is the column number of the constant-head boundary.

Node—is the node number of the constant-head boundary.

Shdfact—is the factor used to calculate the head at the boundary at the start of the stress period from the parameter value. The head is the product of Shdfact and the parameter value.

Ehdfact—is the factor used to calculate the head at the boundary at the end of the stress period from the parameter value. The head is the product of Ehdfact and the parameter value.

ITMP—is a flag and a counter.

If ITMP < 0, non-parameter CHD data from the preceding stress period will be reused.

If ITMP ≥ 0, ITMP is the number of non-parameter constant-head boundaries read for the current stress period.

NP—is the number of parameters in use in the current stress period.

Shead—is the head at the boundary at the start of the stress period.

Ehead—is the head at the boundary at the end of the stress period.

[xyz]—represents the values of the auxiliary variables for a constant-head boundary that have been defined in Item 2. The values of auxiliary variables must be present in each repetition of Items 4 and 6 if they are defined in Item 2. The values must be specified in the order used to define the variables in Item 2.

Pname—is the name of a parameter that is being used in the current stress period. NP parameter names will be read.

Parameter Value (PVAL) File

The Parameter Value File is the file that is specified with "PVAL" as the file type. Parameter values in this file replace parameter values specified in the files where parameters are defined.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. NP

2. PARNAM Parval

NP repetitions of Item 2 are read.

Explanation of Variables Read from the Parameter Value File:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

PARNAM—is the name of a parameter whose value is to be defined. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

Parval—is the parameter value. This value overrides the parameter value specified in the file where the parameter is defined.

DISCRETIZATION FILE

The discretization dataset of MODFLOW-USG has been extended to include a flag TRTOSS as an addition to flags SS and TR which indicate if a stress period is for steady-state or transient flow conditions. This flag TRTOSS indicates that the stress period is a steady-state one, but run in a transient mode for a long time period, till steady-state conditions are achieved. This may be needed for a model that may have difficulty converging for a one-step steady-state solution.

The flag TRTOSS runs the stress period as a transient simulation with adaptive time-stepping and output control as defined in the OC file. However, the stress period is terminated when the rate of change of storage term is below a user defined fraction of the total flow rates in the system. This fraction immediately follows the keyword TRTOSS in the input dataset for each stress period that is treated as transient to steady state.

A TRTOSS stress period should be set up for a long duration (1000s of years) with optimal time stepping using adaptive time-stepping procedures discussed in the Output Control (OC) Package routines and input instructions. That way, the simulation progresses as rapidly as possible and for a long enough duration to ensure it reaches steady state conditions. At every time step of the simulation, MODFLOW-USG computes the ratio of the net rate of change of storage terms to the net total water budget rate (storage plus boundary flow rates) terms. When this ratio is smaller than the user defined fraction, the simulation takes one more time step so that appropriate output can be performed for heads, drawdowns, and fluxes and ends the stress period.

When TRTOSS is used for a stress period, heads and fluxes will be output for the interim time steps to reach steady state, unless the variables in the OC file are appropriately set to only write at the end of a stress period. The default of printing or saving output (heads, drawdowns, fluxes) at the end of a stress period only, is set by using NSTEPS = 0 in the OC file (NSTEPS is otherwise the number of time-steps after which output is written.

Structured Discretization File (DIS)

Discretization information for a structured finite-difference grid is read from the file that is specified by "DIS" as the file type.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. NLAY NROW NCOL NPER ITMUNI LENUNI

2. LAYCBD(NLAY)

3. DELR(NCOL) - U1DREL

Figure 8-1 of the MODFLOW-2005 document illustrates the orientation of DELR and DELC.

4. DELC(NROW) - U1DREL

5. Top(NCOL,NROW) - U2DREL is the top of the model domain.

6. BOTM(NCOL,NROW) - U2DREL is the bottom of each model layer or confining bed.

Item 6 is repeated for each model layer and Quasi-3D confining bed in the grid. Thus, the number of BOTM variables must be NLAY plus the number of Quasi-3D confining beds. The BOTM variables are read in sequence going down from the top of the system. For example, in a 3-layer model with a Quasi-3D confining bed below layer 2, there would be 4 BOTM arrays. The arrays would be the bottom of layer 1, the bottom of layer 2, the bottom of the Quasi-3D confining bed below layer 2, and the bottom of layer 3.

FOR EACH STRESS PERIOD

16. PERLEN NSTP TSMULT Ss/Tr/Trtoss

Explanation of Variables Read from the Discretization File:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NLAY—is the number of layers in the model grid of the groundwater domain.

NROW—is the number of rows in the model grid.

NCOL—is the number of columns in the model grid.

NPER—is the number of stress periods in the simulation.

ITMUNI—indicates the time unit of model data, which must be consistent for all data values that involve time. For example, if "years" is the chosen time unit, then stress-period length, time-step length, transmissivity, and so on, must all be expressed using "years" for their time units. Note that the program will still run even if "undefined" time units are specified because the fundamental equations used in MODFLOW do not require that the time unit be identified; but the user should ensure that consistent units are used for all input data even when ITMUNI indicates an undefined time unit. When the time unit is defined, MODFLOW uses it to print a table of elapsed simulation time:

0 - undefined 3 - hours
1 - seconds 4 - days
2 - minutes 5 - years

LENUNI—indicates the length unit of model data, which must be consistent for all data values that involve length. For example, if "feet" is the chosen length unit, grid spacing, head, hydraulic conductivity, water volumes, and so forth, must all be expressed using "feet" for their length units. Note that the program will still run even if "undefined" length units are specified because the fundamental equations used in MODFLOW do not require that the length unit be identified; but but the user should ensure that consistent units are used for for all input data even when LENUNI indicates an undefined length unit:

0 - undefined
1 - feet
2 - meters
3 - centimeters

LAYCBD—is a flag, with one value for each model layer, that indicates whether or not a layer has a Quasi-3D confining bed below it. 0 indicates no confining bed, and not zero indicates a confining bed. LAYCBD for the bottom layer must be 0.

DELR—is the cell width along rows. Read one value for each of the NCOL columns. This is a multi-value one dimensional variable with one value for each column. (See figure 8-1 of the MODFLOW-2005 document.)

DELC—is the cell width along columns. Read one value for each of the NROW rows. This is a multi-value one dimensional variable with one value for each row. (See figure 8-1 of the MODFLOW-2005 document.)

TOP—is the top elevation of layer 1. For the common situation in which the top layer represents a water-table aquifer, setting Top equal to land-surface elevation may be reasonable.

BOTM—is the bottom elevation of a model layer or a Quasi-3d confining bed.

PERLEN—is the length of a stress period.

NSTP—is the number of time steps in a stress period.

TSMULT—is the multiplier for the length of successive time steps. The length of a time step is calculated by multiplying the length of the previous time step by TSMULT. The length of the first time step, Δt1, is related to PERLEN, NSTP, and TSMULT by the relation

$$\Delta t_1 = PERLEN[TSMULT - 1] / \left[TSMULT^{NSTP} - 1\right]$$

Ss/Tr/Trtoss—is a character variable that indicates whether the stress period is transient or steady state.

- If the value of Ss/Tr is “SS” then the stress period is steady state.
- If the value of Ss/TR is “TR” then the stress period is a transient stress period.
- If the value of Ss/TR is “TRTOSS sf”, then the stress period is running transients to steady-state conditions and will finish the stress period when the storage rate term reduces to below a user defined fraction, “sf” (suggested values are 1e-3 to 1e-6) of the total water budget terms. The fraction immediately follows the keyword, for example, “TRTOSS 1.0e-3”.

Note that the values of NSTP and TSMULT provided here will be superseded when adaptive time stepping is set in the OC file. The PERLEN value entered here will still be used to define the period length.

Unstructured Discretization File (DISU)

Discretization information for unstructured grids is read from the file that is specified by "DISU" as the file type.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. NODES NLAY NJAG IVSD NPER ITMUNI LENUNI IDSYMRD

2. LAYCBD(NLAY)

3. NODELAY(NLAY) - U1DINT

4. Top(NDSLAY) - U1DREL

Repeat Item 4 for each layer in the model grid. Note that there may be different numbers of nodes per layer (NDSLAY) for an unstructured grid.

5. Bot(NDSLAY) - U1DREL

Repeat Item 5 for each layer in the model grid. Note that there may be different numbers of nodes per layer (NDSLAY) for an unstructured grid.

6. Area(NDSLAY) - U1DREL

Item 6 is read only once if IVSD = -1 to indicate that the grid is vertically stacked. Otherwise, repeat Item 6 for each layer in the model grid. Note that there may be different number of nodes per layer (NDSLAY) for an unstructured grid.

7. IAC(NODES) - U1DINT

8. JA(NJAG) - U1DINT

Read item 9 only if IVSD is specified as 1, indicating vertical sub-discretization

9. IVC(NJAG) - U1DINT

Read items 10a and 10b only if ISYMRD=1 for symmetric input of symmetric arrays

10a. CL1(NJAGS) - U1DREL –

10b. CL2(NJAGS) - U1DREL –

Read item 11 only if ISYMRD=0

11. CL12(NJAG) - U1DREL -

12. FAHL(NJAG/NJAGS) - U1DREL -

FOR EACH STRESS PERIOD

13. PERLEN NSTP TSMULT Ss/Tr/Trtoss

Explanation of Variables Read from the Unstructured Discretization File:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NODES—is the number of nodes in the model grid.

NLAY—is the number of layers in the model grid.

NJAG—is the total number of connections of an unstructured grid. NJAG is used to dimension the sparse matrix in a compressed row storage format. For symmetric arrays, only the upper triangle of the matrix may be entered. For that case, the symmetric portion (minus the diagonal terms) is dimensioned as NJAGS = (NJAG – Nodes)/2.

NJAGS—is the total number of non-zero entries for symmetric input of symmetric flow properties between cells. NJAGS = (NJAG – Nodes)/2.

IVSD—is the vertical sub-discretization index. For purposes of this flag, vertical sub-discretization is defined to occur when all layers are not a stacked representation of each other.

If IVSD = 0 there is no sub-discretization of layers within the model domain. That is, grids are not nested in the vertical direction. However, one layer may have a different grid structure from the next due to different sub-gridding structures within each layer.

If IVSD = 1 there could be sub-discretization of layers with vertically nested grids (as shown in Figure 5c in the MODFLOW-USG document) within the domain. For this case, the vertical connection index IVC is required to determine the vertical connections of every node. Otherwise, the vertical connections are internally computed and IVC is not read.

If IVSD = -1 there is no vertical sub-discretization of layers, and further, the horizontal discretization of all layers is the same.. For this case, the cell areas (AREA) are read only for one layer and are computed to be the same for all the stacked layers. A structured finite-difference grid is an example of this condition.

NPER—is the number of stress periods in the simulation.

ITMUNI—indicates the time unit of model data, which must be consistent for all data values that involve time. For example, if "years" is the chosen time unit, then stress-period length, time-step length, transmissivity, and so on, must all be expressed using "years" for their time units. Note that the program will still run even if "undefined" time units are specified because the fundamental equations used in MODFLOW do not require that the time unit be identified; but the user should ensure that consistent units are used for all input data even when ITMUNI indicates an undefined time unit. When the time unit is defined, MODFLOW uses it to print a table of elapsed simulation time:

0 - undefined 3 - hours
1 - seconds 4 - days
2 - minutes 5 - years

LENUNI—indicates the length unit of model data, which must be consistent for all data values that involve length. For example, if "feet" is the chosen length unit, grid spacing, head, hydraulic conductivity, water volumes, and so forth, must all be expressed using "feet" for their length units. Note that the program will still run even if "undefined" length units are specified because the fundamental equations used in MODFLOW do not require that the length unit be identified; but the user should ensure that consistent units are used for all input data even when LENUNI indicates an undefined length unit:

0 - undefined
1 - feet
2 - meters
3 - centimeters

IDSYMRD—is a flag indicating if the finite-volume connectivity information of an unstructured grid is input as a full matrix or as a symmetric matrix in the input file.

If IDSYMRD = 0 finite-volume connectivity information is provided for the full matrix of the porous matrix grid-block connections of an unstructured

grid. The code internally stores only the symmetric portion of this information. This input structure (IDSYMRD=0) is easy to organize but contains unwanted information which is parsed out when the information is stored.

If IDSYMRD = 1 finite-volume connectivity information is provided only for the upper triangular portion of the porous matrix grid-block connections within the unstructured grid. This input structure (IDSYMRD=1) is compact but is slightly more complicated to organize. Only the non-zero upper triangular items of each row are read in sequence for all symmetric matrices.

Note that all symmetric arrays will be handled accordingly.

LAYCBD—is a flag, with one value for each model layer, that indicates whether or not a layer has a Quasi-3D confining bed below it. 0 indicates no confining bed, and not zero indicates a confining bed. LAYCBD for the bottom layer must be 0.

NODELAY—is the number of nodes in each layer.

Top—is the top elevation of the cells.

Bot—is the bottom elevation of the cells.

Area—is the horizontal area of the cells.

IAC—is a matrix indicating the number of connections plus 1 for each node. Note that the IAC array is only supplied for the GWF cells; the IAC array is internally expanded to include CLN or GNC nodes if they are present in a simulation.

JA—is a list of cell number (*n*) followed by its connecting cell numbers (*m*) for each of the *m* cells connected to cell *n*. This list is sequentially provided for the first to the last GWF cell. Note that the cell and its connections are only supplied for the GWF cells and their connections to the other GWF cells. This connectivity is internally expanded if CLN or GNC nodes are present in a simulation. Also note that the JA list input may be chopped up to have every node number and its connectivity list on a separate line for ease in readability of the file. To further ease readability of the file, the node number of the cell whose connectivity is subsequently listed, may be expressed as a negative number the sign of which is subsequently corrected by the code.

IVC—is an index array indicating the direction between a node *n* and all its *m* connections.

IVC = 0 if the connection between *n* and *m* is horizontal.

IVC = 1 if the connecting node *m* is vertically oriented to node *n*.

Note that if the CLN Process is active, the connection between two CLN cells has IVC = 2 and the connection between a CLN cell and a GWF cell has IVC = 3.

CL1— is the perpendicular length between the center of a node (node 1) and the interface between the node and its adjoining node (node 2).

CL2— is the perpendicular length between node 2 and the interface between nodes 1 and 2, and is at the symmetric location of CL1.

CL12—is the array containing CL1 and CL2 lengths, where CL1 is the perpendicular length between the center of a node (node 1) and the interface between the node and its adjoining node (node 2). CL2, which is the perpendicular length between node 2 and the interface between nodes 1 and 2 is at the symmetric location of CL1. The array CL12 reads both CL1 and CL2 in the upper and lower triangular portions of the matrix respectively. Note that the CL1 and CL2 arrays are only supplied for the GWF cell connections and are internally expanded if CLN or GNC nodes exist in a simulation.

FAHL—contains the area of the interface A_{nm} between nodes *n* and *m*.

PERLEN—is the length of a stress period.

NSTP—is the number of time steps in a stress period.

TSMULT—is the multiplier for the length of successive time steps. The length of a time step is calculated by multiplying the length of the previous time step by TSMULT. The length of the first time step, $\Delta t1$, is related to PERLEN, NSTP, and TSMULT by the relation

$$\Delta t_1 = PERLEN[TSMULT - 1] / \left[TSMULT^{NSTP} - 1 \right]$$

Ss/Tr/Trtoss—is a character variable that indicates whether the stress period is transient or steady state.

- If the value of Ss/TR is “SS” then the stress period is steady state.
- If the value of Ss/TR is “TR” then the stress period is a transient stress period.
- If the value of Ss/TR is “TRTOSS sf”, then the stress period is running transients to steady-state conditions and will finish the stress period when the storage rate term reduces to below a user defined fraction, “sf” (suggested values are 1e-3 to 1e-6) of the

total water budget terms. The fraction immediately follows the keyword, for example, "TRTOSS 1.0e-3".

Note that the values of NSTP and TSMULT provided here may be superseded when adaptive time stepping is set in the OC file.

OUTPUT CONTROL PACKAGE FOR SIMULATING FLOW AND TRANSPORT: INPUT INSTRUCTIONS

Output Control with Adaptive Time Stepping – I/O

Input to the Output Control Option of the Groundwater and CLN Flow and Transport Processes is read from the file that is specified as type "OC" in the Name File. If no "OC" file is specified, default output control is used. Under the default, head and overall budget are written to the Listing File at the end of every stress period. If the CLN domain is active, the CLN head and budget are also written to the Listing file when the Groundwater head and budget output is requested. Binary output for the GWF dual domain, and CLN flow Processes, if active, may be to the same head or drawdown file as specified here. Alternatively, the dual domain and CLN flow Processes produce their own output files as discussed in the dual domain and CLN input file documentation (it is preferred that CLN, or dual domain outputs be provided to their own separate output files since many post-processing programs are written to accommodate the files that way). Be it in the same or separate files, the dual domain and CLN outputs are produced whenever the GWF output is produced, as prescribed here. If a transport simulation is conducted, concentrations and mass balance output is provided in a similar manner to output of the flow results. Furthermore, for a multispecies transport simulation, all species concentrations and budgets are written to the same binary output file by default. An option in the transport module input file (MULTIFILE) allows for this to be written separately for each solute species. The default printout format for head, drawdown and concentration is 10G11.4. Output Control data may be specified as words or numeric codes. One of these methods must be used throughout any simulation.

The output control file also provides input for adaptive time stepping parameters, if adaptive time stepping is used in the simulation. Adaptive time stepping is activated by the "option" keyword "ATS" using numeric input and the "option" keyword "ATSA if alphabetic input is provided. Option keywords "NPTIMES" and "NPSTPS" further provide output control when using adaptive time stepping.

Output Control Using Words

Recognized words are shown in bold italics; these words must be entered exactly as shown except that they may be entered in either uppercase or lowercase. Optional parts of lines are shown in brackets. One or more spaces must separate each word or variable, and the total line length must not exceed 199 characters.

FOR EACH SIMULATION

0. [#Text]
Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. Any combination of the following lines:

[**OPTIONS**]–the explanations further below provide the option details. These options can be followed by the following items as part of data item 1.

HEAD PRINT FORMAT IHEDFM
Specifies the format for writing head to the Listing File.

HEAD SAVE FORMAT CHEDFM **[LABEL]**
Specifies the format for writing head to a file other than the Listing File. Omit this line to obtain a binary (unformatted) file. Binary files usually are smaller than text files, but they are not generally transportable among different computer operating systems or different Fortran compilers.

HEAD SAVE UNIT IHEDUN
Specifies the file unit for writing head to a file other than the Listing File.

DRAWDOWN PRINT FORMAT IDDNFM
Specifies the format for writing drawdown to the Listing File.

DRAWDOWN SAVE FORMAT CDDNFM **[LABEL]**
Specifies the format for writing drawdown to a file other than the Listing File. Omit this line to obtain an unformatted (binary) file. Binary files usually are smaller than text files, but they are not generally transportable among different computer operating systems or different Fortran compilers.

DRAWDOWN SAVE UNIT IDDNUN

Specifies the file unit for writing drawdown to a file other than the Listing File.

CONC PRINT FORMAT ISPCFM

Specifies the format for writing concentration of all species to the Listing File.

CONC SAVE FORMAT CSPCFM **[LABEL]**

Specifies the format for writing concentration of all species to a file other than the Listing File. Omit this line to obtain a binary (unformatted) file. Binary files usually are smaller than text files, but they are not generally transportable among different computer operating systems or different Fortran compilers.

CONC SAVE UNIT ISPCUN

Specifies the file unit for writing concentration of all species to a file other than the Listing File.

IBOUND SAVE FORMAT CBOUFM **[LABEL]**

Specifies the format for writing IBOUND to a file.

IBOUND SAVE UNIT IBOUUN

Specifies the file unit for writing IBOUND to a file.

COMPACT BUDGET [AUX or AUXILIARY]

COMPACT BUDGET indicates that the cell-by-cell budget file(s) will be written in a more compact form than is used in the 1988 version of MODFLOW (referred to as MODFLOW-88)(McDonald and Harbaugh, 1988); however, programs that read these data in the form written by MODFLOW-88 will be unable to read the new compact file. If this option is not used, MODFLOW-2005 will write the files using the MODFLOW-88 form. The optional word **AUX** (or ***AUXILIARY***) indicates that auxiliary data that are defined in packages (see input data for the RIV, WEL, DRN, and GHB Packages) should be saved in the budget file along with budget data.

2. TIMOT (nptimes)

Data Item 2 is read only if adaptive time stepping is on, and if the number of print times (NPTIMES) is greater than zero.

FOR EACH TIME STEP FOR WHICH OUTPUT OR ADAPTIVE TIME STEPPING CONTROL IS DESIRED.

3a. **PERIOD** IPEROC **STEP ITSOC [**DDREFERENCE**]**

Data Item 3a is read only if adaptive time stepping is not used. Otherwise, data item 3b is read.

3b. **PERIOD** IPEROC **[**DDREFERENCE**]**

Data Item 3b is read only if adaptive time stepping is used. Otherwise, data item 3a is read.

4. **Any combination of the following lines:**

DELTAT deltat

The keyword ***DELTAT*** is followed by the numeric value *(deltat)* of the time step size with which to begin this stress period. Note that this keyword is used only if adaptive time stepping is on. Also, a value of ***DELTAT*** is required for the first stress period. If a value is not provided for later stress periods, the stress period will begin with a time-step size value equal to the last time step size value from the previous stress period.

TMINAT tminat

The keyword ***TMINAT*** is followed by the numeric value *(tminat)* of the minimum time step size for this stress period. Note that this keyword is used only if adaptive time stepping is on. If a value of ***TMINAT*** is not provided for the first stress period, a default of 1.0e-10 is set. If a value is not provided for later stress periods, the stress period will use the value from the previous stress period.

TMAXAT tmaxat

The keyword ***TMAXAT*** is followed by the numeric value *(tmaxat)* of the maximum time step size for this stress period. Note that this keyword is used only if adaptive time stepping is on. If a value of ***TMAXAT*** is not provided for the first stress period, a default of 1.0e10 is set. If a value is not provided for later stress periods, the stress period will use the value from the previous stress period.

TADJAT tadjat

The keyword ***TADJAT*** is followed by the numeric value *(tadjat)* of the time step size adjustment factor for this stress period. Note that this keyword is used only if adaptive time stepping is on. If a value of ***TADJAT*** is not provided for the first stress period, a default of 2.0 is set. If a value is not provided for later stress periods, the stress period will use the value from the previous stress period. The time step adjustment factor is used as follows.

If convergence is achieved for a time step within one-third the total number of iterations, the time step size is increased by this adjustment factor. If convergence is achieved within two-third the total number of iterations (but more than one-third the total number of iterations), then the time step size is not altered. However, if convergence required greater than two-third of the total number of iterations, then the time step size is decreased by this adjustment factor.

TCUTAT tcutat

The keyword ***TCUTAT*** is followed by the numeric value *(tcutat)* of the time step size cutting factor for this stress period. Note that this keyword is used only if adaptive time stepping is on. If a value of ***TCUTAT*** is not provided for the first stress period, a default of 5.0 is set. If a value is not provided for later stress periods, the stress period will use the value from the previous stress period. The time step cutting factor is used to reduce the time-step size, when convergence is not achieved for a particular time step. In this case, the solution is reattempted with the reduced time step size.

HCLOSE hclose

The keyword ***HCLOSE*** is followed by the numeric value *(hclose)* which is the outer iteration tolerance for this stress period. Note that this keyword is used only if adaptive time stepping is on. A value of ***HCLOSE*** need not be provided here for the first stress period, as it will be taken from the value supplied in the SMS file. However, if provided here for any stress period, the current value will override all previous values. See SMS input instructions for more details on the parameter ***HCLOSE***.

BTOL btol

The keyword ***BTOL*** is followed by the numeric value *(btol)* which is the backtracking tolerance factor for this stress period. Note that this keyword is used only if adaptive time stepping is on. A value of ***BTOL*** need not be provided here for the first stress period, as it will be taken from the value supplied in the SMS file. However, if provided here for any stress period, the current value will override all previous values. See SMS input instructions for more details on the parameter ***BTOL***.

MXITER mxiter

The keyword ***MXITER*** is followed by the numeric value *(mxiter)* which is the maximum number of iterations for this stress period. Note that this keyword is used only if adaptive

time stepping is on. A value of ***MXITER*** need not be provided here for the first stress period, as it will be taken from the value supplied in the SMS file. However, if provided here for any stress period, the current value will override all previous values. See SMS input instructions for more details on the parameter ***MXITER***.

Note that if MXITER is varied in the OC package, it should be used with caution. Specifically, the value set in the SMS package should be larger than any of the values set here in the OC package. This is because the iteration error arrays are dimensioned using MXITER in the SMS package and that dimension should not be exceeded. MXITER can be set at the first iteration in the OC package to the user's requirements, if different from the value in the SMS package.

BOOTSTRAP

The keyword *BOOTSTRAP* is an indication that bootstrapping should be performed for the current stress period onwards from an external file containing head values of a previous simulation. These heads are used at the first iteration as the estimate of HNEW instead of using the HOLD value to help speed up runtimes. This option is active only if the BOOTSTRAPPING option is turned on.

NOBOOTSTRAP

The keyword *NOBOOTSTRAP* is an indication that bootstrapping should not be performed for the current stress period onwards from the external file. Note that the file is still being read to the next time step, only its values are not being used. This option is active only if the BOOTSTRAPPING option is turned on.

BOOTSTRAPSCALE

The keyword *BOOTSTRAPSCALE* is an indication that scaling should be performed for the current stress period onwards when performing bootstrapping. This option is active only if the BOOTSTRAPPING option is turned on.

NOBOOTSTRAPSCALE

The keyword *NOBOOTSTRAPSCALE* is an indication that scaling should not be performed for the current stress period onwards when performing bootstrapping. This option is active only if the BOOTSTRAPPING option is turned on.

PRINT HEAD [list layers if all layers not desired]
Head is written to the Listing File.

PRINT DRAWDOWN [list layers if all layers not desired]
Drawdown is written to the Listing File.

PRINT CONC [list layers if all layers not desired]
Concentration is written to the Listing File.

PRINT BUDGET
Overall volumetric budget is written to the Listing File.

SAVE HEAD [list layers if all layers not desired]
Head is written to a file other than the Listing File.

SAVE DRAWDOWN [list layers if all layers not desired]
Drawdown is written to a file other than the Listing File.

SAVE CONC [list layers if all layers not desired]
Concentration is written to a file other than the Listing File.

SAVE IBOUND [list layers if all layers not desired]
IBOUND is written to a file other than the Listing File. This option is provided to allow changes in IBOUND to be recorded in simulations where IBOUND changes during a simulation.

SAVE BUDGET
Cell-by-cell budget data are written to the files that are designated in the packages that compute budget terms. If solute transport is also simulated, then the SAVE BUDGET keyword also saves the mass flux terms to the appropriate budget files.

Item 2 and one or more Item-4 lines are specified for each time for which output is desired. These lines must be in the order of increasing simulation time. **Note also that the keyword CONCENTRATION may also be used instead of the shorter form CONC when specifying output control using key words.**

Explanation of Variables Read by Output Control Using Words

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

OPTIONS—are optional keywords that activate options:

ATSA indicates that adaptive time stepping will be used in the simulation with output control specified using alphabetic characters.

NPTIMES nptimes: the optional keyword NPTIMES indicates that the following numbers (nptimes) is the number of print times in the simulation. With adaptive time stepping, the time value of a time step is not known apriori and therefore, we cannot determine at which time step, a particular time value will be reached. If printout is required at particular times, the NPTIMES keyword allows input of an array of time values TIMOT (nptimes) at which output is required. The adaptive time stepping routine will adapt the simulation time to exactly match a print time, so computations are performed and output as needed.

NPSTPS npsteps: the optional keyword NPSTPS indicates that the following numbers (npsteps) is the number of steps after which output is provided. When adaptive time stepping is used, the output control items that are otherwise provided for every time step are instead provided for every stress period.

Note that with use of adaptive time stepping, it is appropriate to have output at every time step or every fixed number of time steps during model development, to check how the simulation is performing. During production runs, however, it may be more appropriate to provide time values at which output is desired, so the simulation can adapt and provide computations at those times, for output. Also, by default, output is provided and mass balance information written to the list file, at the end of every stress period. Note further that if both flags NPTIMES and NPSTPS are on, then output is provided according to both flags.

FASTFORWARD ispfast, itsfast, iugfast, [iucfast], [iudfast]: the optional keyword FASTFORWARD indicates that input of **initial conditions of heads** is to be provided from a binary file, which is to be fast-forwarded to the desired stress-period and time-step for input. Boundary condition files are also fast-forwarded up to the desired stress period. Once that input is read, the simulation continues from the next time step or stress period. Currently, three, four or five numbers follow the word FASTFORWARD. The first, **ispfast**,

is the stress period number to which to fast-forward. The second, **itsfast** is the time step number of that stress period, to which to fast-forward. The third, **iugfast** is the unit number on which to open the binary file from which the simulation's initial conditions for heads for the groundwater domain are provided. The fourth number, **iucfast**, is provided only if the CLN domain is simulated and is the unit number on which to open the binary file from which the simulation's initial conditions for heads in the CLN domain are provided. Finally, the fifth number, **iudfast**, is provided only if dual domain flow is simulated and is the unit number on which to open the binary file from which the simulation's initial head conditions for dual domain flow are provided.

This FASTFORWARD option is useful for restarting a flow simulation from somewhere in between, when output has already been provided at the point of restart in a previous simulation.

FASTFORWARDC ispfastc, itsfastc, iugfastc, [iucfastc], [iudfastc], [iumfastc]: the optional keyword FASTFORWARDC indicates that input of **initial conditions of concentration for transport simulations** is to be provided from a binary file, which is to be fast-forwarded to the desired stress-period and time-step for input. Boundary condition files are also fastforwarded up to the desired stress period. Once that input is read, the simulation continues from the next time step or stress period. Currently, three, four or five numbers follow the word FASTFORWARD. The first, **ispfastc**, is the stress period number to which to fast-forward. The second, **itsfastc** is the time step number of that stress period, to which to fast-forward. The third, **iugfastc** is the unit number on which to open the binary file from which the simulation's initial conditions for concentrations in the groundwater domain are provided. The fourth number, **iucfastc**, is provided only if the CLN domain is simulated and is the unit number on which to open the binary file from which the simulation's initial conditions for concentrations in the CLN domain are provided. The fifth number, **iudfastc**, is provided only if dual domain transport is simulated and is the unit number on which to open the binary file from which the simulation's initial concentration conditions for dual domain transport are provided. Finally, the sixth number, **iumfastc**, is provided only if matrix diffusion transport is simulated and is the unit number on which to open the binary file from which the simulation's initial mass conditions for matrix diffusion transport are provided.

This FASTFORWARDC option is useful for restarting a transport simulation from somewhere in between, when output has already been provided at the point of restart in a previous simulation.

BOOTSTRAPPING iugboot, [iucboot], [iudboot]: If the optional keyword BOOTSTRAPPING is used, a bootstrapping procedure is applied for the initial guess of HNEW at the first iteration of a time-step, obtained from external files on unit **iugboot** for groundwater heads, **uicboot** for CLN heads, and **iudboot** for heads in the dual porosity domain. Note that **iucboot** is not read if CLN domain is not present (and may be read as zero if CLN domain bootstrapping is not to be done). Similarly for **iudboot**. The external bootstrapping files should be "HEAD" files in MODFLOW's binary formats (for either structured or unstructured grids) and can be double precision or single precision depending on the DPIN and DPOUT options in the BAS module input. If the BOOTSTRAPPING option is used, the bootstrapping file should be opened in the MODFLOW NAME file as a "DATA(BINARY)" type using the same unit number(s) as **iugboot**, **iucboot** and **iudboot** to indicate that input of **bootstrapping heads will** be provided from binary files. The file may further be identified as OLD in the NAME file to ensure that the file is not overwritten in case unit numbers clash with the output HDS file.

IHEDFM—is a code for the format in which heads will be printed. (Positive values indicate wrap format; negative values indicate strip format.)

0 - 10G11.4	6 - 15F7.4	12 - 10G11.4	18 - 10F6.5
1 - 11G10.	7 - 20F5.0	13 - 10F6.0	19 - 5G12.5
2 - 9G13.6	8 - 20F5.1	14 - 10F6.1	20 - 6G11.4
3 - 15F7.1	9 - 20F5.2	15 - 10F6.2	21 - 7G9.2
4 - 15F7.2	10 - 20F5.3	16 - 10F6.3	
5 - 15F7.3	11 - 20F5.4	17 - 10F6.4	

CHEDFM—is a character value that specifies the format for saving heads, and can only be specified if the word method of output control is used. The format must contain 20 characters or less and must be a valid Fortran format that is enclosed in parentheses. The format must be enclosed in apostrophes if it contains one or more blanks or commas. The

optional word ***LABEL*** after the format is used to indicate that each layer of output should be preceded with a line that defines the output (simulation time, the layer being output, and so forth). If there is no line specifying CHEDFM, then heads are written to a binary (unformatted) file. Binary files are usually more compact than text files, but they are not generally transportable among different computer operating systems or different Fortran compilers.

IHEDUN—is the unit number on which head will be saved.

IDDNFM—is a code for the format in which drawdown will be printed. The codes are the same as for IHEDFM.

ISPCFM—is a code for the format in which concentrations of all species will be printed. The codes are the same as for IHEDFM.

CSPCFM—is a character value that specifies the format for saving concentrations, and can only be specified if the word method of output control is used. The format must contain 20 characters or less and must be a valid Fortran format that is enclosed in parentheses. The format must be enclosed in apostrophes if it contains one or more blanks or commas. The optional word ***LABEL*** after the format is used to indicate that each layer of output should be preceded with a line that defines the output (simulation time, the layer being output, and so forth). If there is no line specifying CSPCFM, then concentrations are written to a binary (unformatted) file. Binary files are usually more compact than text files, but they are not generally transportable among different computer operating systems or different Fortran compilers.

ISPCUN—is the unit number on which concentrations will be saved.

CDDNFM—is a character value that specifies the format for saving drawdown, and can only be specified if the word method of output control is used. The format must contain 20 characters or less and must be a valid Fortran format that is enclosed in parentheses. The format must be enclosed in apostrophes if it contains one or more blanks or commas. The optional word LABEL after the format is used to indicate that each layer of output should be preceded with a line that defines the output (simulation time, the layer being output, and so forth). If there is no line specifying CDDNFM, then drawdown is written to a binary (unformatted) file. Binary files are usually more compact than text files, but they are not

generally transportable among different computer operating systems or different Fortran compilers.

IDDNUN—is the unit number on which drawdowns will be saved.

CBOUFM—is a character value that specifies the format for saving IBOUND, and can only be specified if the word method of output control is used. The format must contain 20 characters or less and must be a valid Fortran format that is enclosed in parentheses. The format must be enclosed in apostrophes if it contains one or more blanks or commas. The optional word LABEL is used to indicate that each layer of output should be preceded with a line that defines the output (simulation time, the layer being output, and so forth). If there is no line specifying CBOUFM, then IBOUND is written using format (20I4). IBOUND is never written as a binary (unformatted) file.

IBOUUN—is the unit number on which IBOUND will be saved.

TIMOT—is the array of time values at which output is requested. There are NPTIMES entries in the TIMOT array. Note that the first time step (DELTAT) of a stress period should not be larger than the next value in the TIMOT array. Otherwise, the code will print an error and stop.

IPEROC—is the stress period number at which output is desired.

ITSOC—is the time step number (within a stress period) at which output is desired.

DDREFERENCE—keyword indicating that the heads at the associated stress period and time step are to be used as the reference heads for calculating drawdown for all subsequent time steps up to the next occurrence of DDREFERENCE. Prior to the first occurrence (if any) of DDREFERENCE the initial heads (STRT) will be used as the reference heads for calculating drawdown.

Example Output Control Input Using Words

```
HEAD PRINT FORMAT 15
HEAD SAVE FORMAT (20F10.3) LABEL
HEAD SAVE UNIT 30
COMPACT BUDGET
```

```
DRAWDOWN PRINT FORMAT 14
PERIOD 1 STEP 1
    PRINT HEAD 2 6
    PRINT DRAWDOWN
    PRINT BUDGET
    SAVE BUDGET
    SAVE HEAD
    SAVE CONCENTRATION
PERIOD 1 STEP 7
    SAVE HEAD 1 3 5
    PRINT DRAWDOWN
    SAVE BUDGET
PERIOD 2 STEP 5
    PRINT HEAD
    PRINT BUDGET
    SAVE BUDGET
    SAVE HEAD
```

Note that the first line cannot be blank, but after the first line blank lines are ignored when the word method is used to specify Output Control data. Indented lines are allowed because of the use of free format input.

Example Output Control with Adaptive Time Stepping Input Using Words

```
ATSA NPTIMES 2 NPSTPS 20 BOOTSTRAPPING 45 46
    5.0E3 3.13E8            ! these are the 2 print times in TIMOT
    HEAD SAVE UNIT 30
    HEAD PRINT FORMAT 0
    DRAWDOWN SAVE UNIT 31
    DRAWDOWN PRINT FORMAT 0
PERIOD 1
    DELTAT 5.0E2
    TMAXAT 5.0E5
    SAVE HEAD
```

SAVE DRAWDOWN
SAVE BUDGET
PRINT BUDGET
BOOTSTRAP
BOOTSTRAPSCALE
PERIOD 2
DELTAT 3600.00
TADJAT 2.5
SAVE HEAD
SAVE DRAWDOWN
PRINT BUDGET
PERIOD 3
SAVE HEAD
SAVE DRAWDOWN
PRINT BUDGET
PERIOD 120
SAVE HEAD
SAVE DRAWDOWN
PRINT BUDGET

Note that the first line cannot be blank, but after the first line blank lines are ignored when the word method is used to specify Output Control data. Indented lines are allowed because of the use of free format input.

Output Control Using Numeric Codes

All variables are free format if the word FREE is specified in Item 1 of the Basic Package input file; otherwise, the variables all have 10-character fields.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. **IHEDFM IDDNFM IHEDUN IDDNUN ISPCFM ISPCUN [OPTIONS]**

2. **TIMOT (nptimes)**
   Data Item 2 is read only if adaptive time stepping is on, and if the number of print times (NPTIMES) is greater than zero.

   Item 3 is read for each time step if adaptive time stepping is not used. If adaptive time stepping is used, item 3 is read for each stress period.

3. **DELTAT TMINAT TMAXAT TADJAT TCUTAT**
   Data Item 3 is read only if adaptive time stepping is on.

4. **INCODE IHDDFL IBUDFL ICBCFL ISPCFL**

5. **Hdpr Ddpr Hdsv Ddsv Cnpr Cnsv**
   (Item 3 is read 0, 1, or NLAY times, depending on the value of INCODE.)

Explanation of Variables Read by Output Control Using Numeric Codes

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

IHEDFM—is a code for the format in which heads will be printed. See the description above in the explanation of variables read by output control using words.

IDDNFM—is a code for the format in which drawdowns will be printed. The codes are the same as for IHEDFM.

IHEDUN—is the unit number on which heads will be saved.

IDDNUN—is the unit number on which drawdowns will be saved.

ISPCFM—is a code for the format in which concentrations will be printed. The codes are the same as for IHEDFM.

ISPCUN—is the unit number on which concentrations will be saved.

OPTIONS—are optional keywords that activate options:

ATS indicates that adaptive time stepping will be used in the simulation with output control specified using numeric characters.

NPTIMES nptimes: the optional keyword NPTIMES indicates that the following numbers (nptimes) is the number of print times in the simulation. With adaptive time stepping, the time value of a time step is not known apriori and therefore, we cannot determine at which time step, a particular time value will be reached. If printout is required at particular times, the NPTIMES keyword allows input of an array of time values TIMOT(nptimes) at which output is required. The adaptive time stepping routine will adapt the simulation time to exactly match a print time so computations are performed and output as needed.

NPSTPS npsteps: the optional keyword NPSTPS indicates that the following numbers (npsteps) is the number of steps after which output is provided. When adaptive time stepping is used, the output control items that are otherwise provided for every time step are instead provided for every stress period.

Note that with use of adaptive time stepping, it is appropriate to have output at every time step or every fixed number of time steps during model development, to check how the simulation is performing. During production runs, however, it may be more appropriate to provide time values at which output is desired, so the simulation can adapt and provide computations at those times, for output.

BOOTSTRAPPING iugboot, [iucboot], [iudboot]: If the optional keyword BOOTSTRAPPING is used, a bootstrapping procedure is applied for the initial guess of HNEW at the first iteration of a time-step, obtained from external files on unit **iugboot** for groundwater heads, **uicboot** for CLN heads, and **iudboot** for heads in the dual porosity domain. Note that **iucboot** is not read if CLN domain is not present (and may be read as zero if CLN domain bootstrapping is not to be done). Similarly for **iudboot**. The external bootstrapping files should be "HEAD" files in MODFLOW's binary formats (for either structured or unstructured grids) and can be double precision or single precision depending on the DPIN and DPOUT options in the BAS module input. If the BOOTSTRAPPING option is used, the bootstrapping file should be opened in the MODFLOW NAME file as a "DATA(BINARY)" type using the same unit number(s) as **iugboot**, **iucboot** and **iudboot** to indicate that input of **bootstrapping heads will** be provided from binary files. The file may

further be identified as OLD in the NAME file to ensure that the file is not overwritten in case unit numbers clash with the output HDS file.

TIMOT—is the array of time values at which output is requested. There are NPTIMES entries in the TIMOT array. Note that the first time step (DELTAT) of a stress period should not be larger than the next value in the TIMOT array. Otherwise, the code will print an error and stop.

DELTAT—is the time step size with which to begin this stress period.

TMINAT—is the minimum time step size for this stress period.

TMAXAT—is the maximum time step size for this stress period.

TADJAT—is the time step size adjustment factor this stress period. The time step adjustment factor is used as follows. If convergence is achieved for a time step within one-third of the total number of iterations, the time step size is increased by this adjustment factor. If convergence is achieved within two-third of the total number of iterations (but more than one-third the total number of iterations), then the time step size is not altered. However, if convergence required greater than two-third of the total number of iterations, then the time step size is decreased by this adjustment factor.

TCUT—is the time step size cutting factor this stress period. The time step cutting factor is used to reduce the time-step size, when convergence is not achieved for a particular time step. In this case, the solution is reattempted with the reduced time step size.

IBOOT—is a flag indicating if the time steps of the current stress period are to be bootstrapped.

IBOOT = 0, no, use HNEW from HOLD for the first iteration of every time step in this stress period.

IBOOT = 1, yes, use HNEW from external binary file with file type of BTS in the NAME file. Note that the external binary file should have compatible time stepping through all stress periods with the current simulation.

IBOOTSCALE—is a flag indicating if scaling is applied to the change as per ratio of actual change versus bootstrapped change for the previous time-step.

IBOOTSCALE = 0, no, scaling is applied.

IBOOT = 1, yes, scaling is applied.

INCODE—is the code for reading Item 3.

If **INCODE < 0**, Item 3 flags are used from the last time step. Item 3 is not read.

If **INCODE = 0**, all layers are treated the same way. Item 3 will consist of one line.

If **INCODE > 0**, Item 3 will consist of one line for each layer.

IHDDFL—is a head and drawdown output flag. This flag allows Item 3 flags to be specified in an early time step and then used or not used in subsequent time steps. Thus, using IHDDFL to avoid resetting Item 3 flags every time step may be possible.

If **IHDDFL = 0**, no heads or drawdowns will be printed or saved regardless of which Item 3 flags are specified.

If **IHDDFL ≠ 0**, heads and drawdowns will be printed or saved according to the Item 3 flags.

IBUDFL—is a budget print flag.

If **IBUDFL = 0**, overall volumetric budget will not be printed.

If **IBUDFL ≠ 0**, overall volumetric budget will be printed.

ICBCFL—is a flag for writing cell-by-cell flow data. Note that if transport is simulated, this flag also controls output of cell-by-cell mass flux data.

If **ICBCFL = 0**, cell-by-cell flow terms are not written to any file.

If **ICBCFL ≠ 0**, cell-by-cell flow terms are written to the LIST file or a budget file depending on flags set in the component of flow packages, that is, IWELCB, IRCHCB, and so forth.

ISPCFL—is a concentration output flag. This flag allows Item 3 flags to be specified in an early time step and then used or not used in subsequent time steps. Thus, using ISPCFL to avoid resetting Item 3 flags every time step may be possible.

If **ISPCFL = 0**, no concentrations will be printed or saved regardless of which Item 3 flags are specified.

If **ISPCFL ≠ 0**, concentrations will be printed or saved according to the Item 3 flags.

Hdpr—is the output flag for head printout.

If **Hdpr = 0**, head is not printed for the corresponding layer.

If **Hdpr ≠ 0**, head is printed for the corresponding layer.

Ddpr—is the output flag for drawdown printout.

If **Ddpr = 0**, drawdown is not printed for the corresponding layer.

If **Ddpr ≠ 0**, drawdown is printed for the corresponding layer.

Hdsv—is the output flag for head save.

If **Hdsv = 0**, head is not saved for the corresponding layer.

If **Hdsv ≠ 0**, head is saved for the corresponding layer.

Ddsv—is the output flag for drawdown save.

If **Ddsv = 0**, drawdown is not saved for the corresponding layer.

If **Ddsv ≠ 0**, drawdown is saved for the corresponding layer.

Cnpr—is the output flag for concentration printout.

If **Cnpr = 0**, concentration is not printed for the corresponding layer.

If **Cnpr ≠ 0**, concentration is printed for the corresponding layer.

Cnsv—is the output flag for concentration save.

If **Cnsv = 0**, concentration is not saved for the corresponding layer.

If **Cnsv ≠ 0**, concentration is saved for the corresponding layer.

INPUT INSTRUCTIONS FOR ARRAY READING UTILITY SUBROUTINES

The array reading utility subroutines provide a common way for all packages to read variables that have multiple values. The term “array” is simply a programming term for a variable that contains multiple values. There are three subroutines: U2DREL, U2DINT, and U1DREL. U2DREL reads real two-dimensional variables, U2DINT reads integer two-dimensional variables, and U1DREL reads real one-dimensional variables. A variation on U2DREL and U1DREL are the U2DREL8 and U1DREL8 subroutines which are used to read real *8 (double precision) arrays. Their specific utility is in reading binary files which were generated in double precision from a previous simulation.

All of these subroutines work similarly. They read one array-control line and, optionally, a data array in a format specified on the array-control line. Several alternate structures for the control line are provided. The original fixed-format control lines work as documented in McDonald and Harbaugh (1988), and four free-format versions have been added. The free-format versions are described first because they are easier to use.

Free-format control lines for array readers

Values in bold italics are keywords that can be specified as uppercase or lowercase. Each control line is limited to a length of 199 characters.

1. **CONSTANT** CNSTNT

All values in the array are set equal to CNSTNT.

2. **INTERNAL** CNSTNT FMTIN IPRN

The individual array elements will be read from the same file that contains the control line.

3. **EXTERNAL** Nunit CNSTNT FMTIN IPRN

The individual array elements will be read from the file unit number specified by Nunit. The name of the file associated with this file unit must be contained in the Name File.

4. **OPEN/CLOSE** FNAME CNSTNT FMTIN IPRN

The array will be read from the file whose name is specified by FNAME. This file will be opened on unit 99 just prior to reading the array and closed immediately after the array is read. This file should not be included in the Name File. A file that is read using this control line can contain only a single array.

Fixed-format control line for array readers

A fixed-format control line contains the following variables:

LOCAT CNSTNT FMTIN IPRN

These variables are explained below. LOCAT, CNSTNT, and IPRN are 10-character numeric fields. For U2DREL and U1DREL, CNSTNT is a real number. For U2DINT, CNSTNT is an integer and must not include a decimal. FMTIN is a 20-character text field. All four variables are always read when the control line is fixed format; however, some of the variables are unused in some situations. For example when LOCAT = 0, FMTIN and IPRN are not used.

CNSTNT—is a real-number constant for U2DREL and U1DREL, and an integer constant for U2DINT. If the array is being defined as a constant, CNSTNT is the constant value. If individual elements of the array are being read, the values are multiplied by CNSTNT after they are read. CNSTNT, when used as a multiplier and specified as 0, is changed to 1.

FMTIN—is the format for reading array elements. The format must contain 20 characters or less. The format must either be a standard Fortran format that is enclosed in parentheses, "(FREE)" which indicates free format, or "(BINARY)" which indicates binary (unformatted) data. When using a free-format control line, the format must be enclosed in apostrophes if it contains one or more blanks or commas. A binary file that can be read by MODFLOW may be created in only two ways. The first way is to use MODFLOW to create the file by saving heads in a binary file. This is commonly done when the user desires to use computed heads from one simulation as initial heads for a subsequent simulation. The other way to create a binary file is to write a special program that generates a binary file, and compile this program using a Fortran compiler that is compatible with the compiler used to compile MODFLOW. "(FREE)" and "(BINARY)" can only be specified in free-format control lines. Also, "(BINARY)" can be specified only when using U2DREL or U2DINT, and only when the

control line is EXTERNAL or OPEN/CLOSE. When the "(FREE)" option is used, be sure that all array elements have a non-blank value and that a comma or at least one blank separates adjacent values.

IPRN—is a flag that indicates whether the array being read should be written to the Listing File after the array has been read and a code for indicating the format that should be used when the array is written. The format codes are different for each of the three array-reading subroutines as shown below. IPRN is set to zero when the specified value exceeds those defined. If IPRN is less than zero, the array will not be printed.

IPRN	U2DREL	U2DINT	U1DREL
0	10G11.4	10I11	10G12.5
1	11G10.3	60I1	5G12.5
2	9G13.6	40I2	
3	15F7.1	30I3	
4	15F7.2	25I4	
5	15F7.3	20I5	
6	15F7.4	10I11	
7	20F5.0	25I2	
8	20F5.1	15I4	
9	20F5.2	10I6	
10	20F5.3		
11	20F5.4		
12	10G11.4		
13	10F6.0		
14	10F6.1		
15	10F6.2		
16	10F6.3		
17	10F6.4		
18	10F6.5		
19	5G12.5		

20	6G11.4		
21	7G9.2		

Nunit—is the unit for reading the array when the ***EXTERNAL*** free-format control line is used.

LOCAT—indicates the location of the array values for a fixed-format array control line. If LOCAT = 0, all elements are set equal to CNSTNT. If LOCAT > 0, it is the unit number for reading formatted lines using FMTIN as the format. If LOCAT < 0, it is the unit number for binary (unformatted) lines, and FMTIN is ignored. Also, when LOCAT is not 0, the array values are multiplied by CNSTNT after they are read.

Examples of Free-Format Control Lines

The following examples use free-format control lines for reading an array. The example array is a real array consisting of 4 rows with 7 columns per row:

CONSTANT 5.7	This sets an entire array to the value "5.7".
INTERNAL 1.0 (7F4.0) 3 1.2 3.7 9.3 4.2 2.2 9.9 1.0 3.3 4.9 7.3 7.5 8.2 8.7 6.6 4.5 5.7 2.2 1.1 1.7 6.7 6.9 7.4 3.5 7.8 8.5 7.4 6.8 8.8	This reads the array values from the file that contains the control line. Thus, the values immediately follow the control line.
EXTERNAL 52 1.0 (7F4.0) 3	This reads the array from the formatted file opened on unit 52.
EXTERNAL -47 1.0 (BINARY) 3	This reads the array from the binary file opened on unit 47. Note the negative unit number representing binary file input.

OPEN/CLOSE test.dat 1.0 (7F4.0) 3	This reads the array from the file named "test.dat". Note that test.dat needs to be an ASCII file and cannot be binary if this format is used to access the file.

Input Instructions for List Utility Subroutine (ULSTRD)

Subroutine ULSTRD reads lists that are any number of repetitions of an input item that contains multiple variables. Examples of packages that make use of this subroutine are the General-Head Boundary, Drain, River, and Well Packages.

1. [EXTERNAL IN] or [OPEN/CLOSE FNAME]

If Item 1 is not included, then the list is read from the package file. Item 1 must begin with the keyword “EXTERNAL” or the keyword “OPEN/CLOSE” (not both).

2. [SFAC Scale]

3. List

Explanation of Variables Read by the List Utility Subroutine:

IN—is the unit number for a file from which the list will be read. The name of the file associated with this file unit must be contained in the Name File, and its file type must be “DATA” in the Name File.

FNAME—is the name of a file from which the list will be read. This file will be opened on unit 99 just before reading the list and closed immediately after the list is read. This file should not be included in the Name File.

Scale—is a scale factor that is multiplied times the value of one or more variables within every line of the list. The input instructions that define a list, which will be read by ULSTRD, should specify the variables to which SFAC applies. If Item 2 is not included, then Scale is 1.0. If Item 2 is included, it must begin with the keyword “SFAC.” The values of the list variables that are printed to the listing file include the effect of Scale.

List—is a specified number of lines of data in which each line contains a specified number of variables. The first three variables are always layer, row, and column. The other fields vary according to which package is calling this subroutine.

DESCRIPTION OF BINARY OUTPUT FILES

The format of the binary output files written by MODFLOW-USG depends on whether or not the model is structured or unstructured. If the name file contains a "DIS" file type, then the model is structured; if the name file contains a "DISU" file type, then the model is unstructured. If the model is structured, then the format of the binary output files written by MODFLOW-USG is the same as the format used by MODFLOW-2005. If the model is unstructured, then the format of the binary files is different from the MODFLOW-2005 format.

Variable names that begin with the letters A to H and O to Z are of type REAL. If MODFLOW-USG is compiled using a compiler switch that sets all REAL variables to DOUBLE PRECISION, then all REAL output values will be of type DOUBLE PRECISION. Otherwise, all REAL output values will be of single precision. There is also an option in USG to write binary file output in double precision for heads, concentrations and drawdowns. Variables that begin with the letters I to N are integers, and are written to the output file as integers. Some variables are character strings and are indicated as so in the following descriptions.

The file formats for head, concentration and drawdown data and for cell-by-cell flow data are described for both structured and unstructured grids in the following sections. The frequency of output and the types of output files that are created is described in the Output Control Option and in the individual package input files.

Structured Head, Concentration, (Temperature) and Drawdown File Format

For each stress period, time step, and layer for which data are saved to the binary output file, the following two records are written:

Record 1: KSTP,KPER,PERTIM,TOTIM,TEXT,NCOL,NROW,ILAY

Record 2: ((DATA(J, I), J=1,NCOL),I=1,NLAY)

where

KSTP is the time step number (real);

KPER is the stress period number (real);

PERTIM is the time value for the current stress period (real);

TOTIM is the total simulation time (real);

TEXT is a character string (character*16);

NCOL is the number of columns (integer);

NROW is the number of rows (integer);

ILAY is the layer number (integer); and

DATA is either the head or drawdown data (real array).

In the present MODFLOW-USG version, TEXT can be “HEAD”, “CONC”, “TMPR” or “DRAWDOWN”. CONC and TMPR represent solute concentration and temperature. If there are multiple mobile components, then the concentration for each of the components is identified by the species number. Thus, if there are three solute species, the output text will be “CONC01”, “CONC02”, and “CONC03”. ***Note that the real variables are written as real*8 (double precision) when the option for writing heads, concentrations or drawdowns in double precision format is selected. This includes the variables PERTIM and TOTIM and the array DATA***.

Unstructured Head, Concentration, (Temperature), and Drawdown File Format

For each stress period, time step, and layer that is saved to the binary output file, the following two records are written:

Record 1: KSTP,KPER,PERTIM,TOTIM,TEXT,NSTRT,NNDLAY,ILAY

Record 2: (DATA(N), N=NSTRT,NNDLAY)

where

KSTP is the time step number (real);

KPER is the stress period number (real);

PERTIM is the time value for the current stress period (real);

TOTIM is the total simulation time (real);

TEXT is a character string (character*16);

NSTRT is the starting cell number for the layer (real);

NNDLAY is the cell number of the last cell in the layer (inteter);

ILAY is the layer number (integer); and

DATA is either the unstructured head or drawdown data (real).

In the present MODFLOW-USG version, TEXT can be “HEADU”, “DRAWDOWNU”, “CONC”, “TMPR”, “CLN HEADS”, “CLN DRAWDOWN”, “CLN CONC”, or “CLN TMPR”. For multiple mobile components, the concentration for each of the components is identified by the species number. Thus, if there are three solute species, the output text will be “CONC01”, “CONC02”, and “CONC03”. The “U” character at the end of “HEADU” and “DRAWDOWNU” indicate that the grid is unstructured. ***Note that the real variables are written as real*8 (double precision) when the option for writing heads, concentrations or drawdowns in double precision format is selected. This includes the variables PERTIM and TOTIM and the array DATA***.

Structured Cell-by-Cell Flow File

The format for the cell-by-cell flow file is more complicated than the format for the head and drawdown data. The cell-by-cell flow file can be written in the regular legacy style, in which three-dimensional arrays are written for all packages, even if most of the values are zero. The cell-by-cell flow file can also be written in the compact budget style, which is the preferred format, because the cell-by-cell flow file is much smaller and because additional information, such as timing information and auxiliary variable values, is written. The compact budget style is activated by adding “COMPACT BUDGET” to the output control input file.

For each stress period and time step that is saved to the binary output file, the following records are written:

Record 1: KSTP,KPER,TEXT,NCOL,NROW,NLAY

If NLAY > 0: *The budget data is written in legacy style.*

Record 2: (((DATA(J,I,K),J=1,NCOL),I=1,NROW),K=1,NLAY)

If NLAY < 0: *The budget data is written in the compact budget style.*

Record 2: IMETH,DELT,PERTIM,TOTIM

If IMETH=1: *The budget data is full grid array.*

Record 3: (((DATA(J,I,K),J=1,NCOL),I=1,NROW),K=1,NLAY)

If IMETH=2: *The budget data is a list.*

Record 3: NLIST

Record 4: ((NODE(N),Q(N)),N=1,NLIST)

If IMETH=3: *The budget data is a two-dimensional array that has a layer indicator array.*

Record 3: ((ILAYER(J,I),J=1,NCOL),I=1,NROW)

Record 4: ((DATA(J, I), J=1,NCOL),I=1,NLAY)

If IMETH=4: *The budget data is a two-dimensional array that applies to layer 1.*

Record 3: ((DATA(J, I), J=1,NCOL),I=1,NLAY)

If IMETH=5: *The budget data is a list with auxiliary data.*

Record 3: NVAL

Record 4: (AUXTXT(N),N=1,NVAL-1)

Record 5: NLIST

Record 6: ((NODE(N),(DATA(I,N),I=1,NVAL)),N=1,NLIST)

Where:

KSTP is the time step number (real);

KPER is the stress period number (real);

TEXT is a character string (character*16) name of the budget term;

NCOL is the number of columns (integer);

NROW is the number of rows (integer);

NLAY is the layer number (integer);

IMETH is a code that specifies the form of the remaining data (integer);

DELT is the length of the timestep (real);

PERTIM is the time value for the current stress period (real);

TOTIM is the total simulation time (real);

DATA is a two- or three-dimensional array of the budget values (real). When IMETH=5, the budget value for each list entry is contained in the first DATA column;

NLIST is the number of values in the following list (integer);

NODE is the one-dimensional node number (integer);

Q is the budget value (real);

ILAYER is an two-dimensional layer indicator array corresponding to the subsequent DATA array (integer);

NVAL is the number of values for each list entry, which is the number of auxiliary values plus 1 (integer); and

AUXTXT is an array of size NVAL - 1 containing character*16 text names for each auxiliary variable.

Note that there is no option for writing budget terms in double precision formats. If that is required then the entire code may be compiled using the double precision compiler option.

Unstructured Cell-by-Cell Flow File

For unstructured grids, the cell-by-cell flow file can also be written in the legacy style; however, in this case, the budget arrays are one-dimensional with the size equal to the number of nodes, in contrast to the three-dimensional budget arrays written for structured grids. Except for budget terms corresponding to flows between cells and storage, most of the budget terms will be zero for typical applications. The cell-by-cell flow file can also be written in the compact budget style for unstructured grids, which is the preferred format, because the cell-by-cell flow file is much smaller and because additional information, such as timing information and auxiliary variable values, is written.

For each stress period and time step for which budget data are requested to be saved to the binary output file, the following records are written:

Record 1: KSTP,KPER,TEXT,NVAL,1,ICODE

If ICODE > 0: *The budget data is written in legacy style.*

Record 2: (DATA(I),I=1,NVAL)

If ICODE = -1: *The budget data is written in the compact budget style.*

Record 2: IMETH,DELT,PERTIM,TOTIM

If IMETH=1: *The budget data is full grid array*.

Record 3: (DATA(I),I=1,NVAL)

If IMETH=2: *The budget data is a list.*

Record 3: NLIST

Record 4: ((NODE(N),Q(N)),N=1,NLIST)

If IMETH=3: *The budget data is a one-layer array that has a one-dimensional node indicator array*.

Record 3: (INODE(I),I=1,NVAL)

Record 4: (DATA(I),I=1,NVAL)

If IMETH=4: *The budget data is a one-dimensional array that applies to layer 1.*

Record 3: (DATA(I),I=1,NVAL)

If IMETH=5: *The budget data is a list with auxiliary data.*

Record 3: NDAT

Record 4: (AUXTXT(N),N=1,NDAT-1)

Record 5: NLIST

Record 6: ((NODE(N),(DATA(I,N),I=1,NDAT)),N=1,NLIST)

where

KSTP is the time step number (real);

KPER is the stress period number (real);

TEXT is a character string (character*16) name of the budget term;

NVAL is the number of data values (unless it is a list, then NVAL is the number of nodes in the grid) (integer);

ICODE indicates whether the file is legacy or compact style (integer);

IMETH is a code that specifies the form of the remaining data (integer);

DELT is the length of the timestep (real);

PERTIM is the time value for the current stress period (real);

TOTIM is the total simulation time (real);

DATA is a one- or two-dimensional array of the budget values. When IMETH=5, the budget value for each list entry is contained in the first DATA column (real);

NLIST is the number of values in the following list (integer);

NODE is the node number indicating the location of the stress (integer);

Q is the budget value (real);

INODE is a one-dimensional node indicator array corresponding to the subsequent DATA array (integer);

NDAT is the number of values for each list entry, which is the number of auxiliary values plus 1 (integer). Note that the first data value is the budget term. The remaining values in DATA are the values for the auxiliary variables.

AUXTXT is an array of size NDAT - 1 containing character*16 text names for each auxiliary variable.

MODFLOW-USG writes a special record for flow between connected cells. This record has a TEXT identifier equal to “FLOW JA FACE”. For this record, NVAL is equal to NJAG, which is the total number of connections **plus 1** for all of the groundwater cell connections. Therefore, this budget record corresponds to the JA array. A value of zero is written to the node positions in the “FLOW JA FACE” record. Also terms related to the CLN domain will have a CLN preceding the term (CLN HEAD, for example).

BLOCK-CENTERED FLOW (BCF) PACKAGE INPUT WITH UNSATURATED FLOW

Input for the Block-Centered Flow (BCF) Package is read from the file that is type "BCF6" in the Name File. Options in addition to MODFLOW-USG capabilities include:

- Option to compute compressible storage with an alternate formulation (ALTSTO). Instead of compressible storage changing from zero to full with grid block saturation, it is smoothly applied over only a small distance from the top of a grid-block. This is the more conventional application of a storage coefficient but may have more numerical difficulties than the original formulation. No further input is required when using this option aside from calling it out in the “options” section.

- Solution of 3-dimensional Richards’ Equation for unsaturated zone domain. This option can be invoked in the BAS file for the whole domain or can be applied here on a layer-by-layer basis. For instance, the top few layers of a model may be simulated as “unsaturated”, with the remaining layers below being “unconfined”. Text in this color may be skipped if Richards’ equation is not solved by the model.

The BCF Package is an alternative to the LPF Package. Both packages should not be used simultaneously.

FOR EACH SIMULATION

If UNSTRUCTURED option is used, then read item 1a

1a. IBCFCB HDRY IWDFLG WETFCT IWETIT IHDWET IKVFLAG IKCFLAG [OPTIONS]

These EIGHT variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the variables all have 10-character fields.

Otherwise, if UNSTRUCTURED option is not used then read item 1b for structured input

1b. IBCFCB HDRY IWDFLG WETFCT IWETIT IHDWET **IKVFLAG [OPTIONS]**

These seven variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the variables all have 10-character fields.

Read item 1c and d below, only if the TABRICH option is invoked above, to indicate tabular input of moisture retention and relative permeability curves for Richards' equation solution in the unsaturated zone.

1c. IUZONTAB(NODES) -- U1DINT

1d. RETCRVS(HC, SAT,Kr)

Item 1d is the tabular input of moisture retention parameters of each soil type and is repeated "**nutabrows**" times for all the rows of the table, which is then repeated "**nuzones**" times for each soil type in the catalogue.

2. Ltype(NLAY)

   Read one value for each layer. These values are free format if the word FREE is specified in Item 1 of the Basic Package input file; otherwise, the values are read using fixed format fields that are each 2 characters wide with 40 values per line. Use only as many lines as required for the number of model layers.

   Read item 3 for structured grids. For unstructured grids, read item 3 only if IKCFLAG = 0 for nodal input of hydraulic conductivities.

3. TRPY(NLAY) -- U1DREL

   If UNSTRUCTURED option is used then read item 4 if any layer is anisotropic (i.e., if any of TRPY is not equal to one.

4. [ANGLEX(NJAG)] – U1DREL.

If UNSTRUCTURED option is used then read items 5 through 15. A subset of the following one-dimensional variables is used to describe each node. The variables needed for each node depend on the layer-type code of the layer in which the node resides (LAYCON, which is defined as part of the Item-2 Ltype), whether the simulation has any transient stress periods (at least one stress period defined in the Discretization File specifies Ss/Tr as "TR"), and if the wetting capability is active (IWDFLG not 0). Unneeded variables must be omitted. In no situation will all variables be required.

The required variables for Items 5-10 for layer 1 are read first; then the variables for layer 2 and so forth. Also note that there may be different number of nodes per layer (NDSLAY) for an unstructured grid.

5. [Sf1(NDSLAY)] – U1DREL If there is at least one transient stress period.

   If IKCFLAG=0 for nodal input of conductivities, then read items 6 through 8

   If LAYCON is 0 or 2 (see Ltype), read transmissivity of the node into item 6a.

6a. [Tran(NDSLAY)] – U1DREL.

   Otherwise, if LAYCON is 1 or 3 or 4 (see Ltype), read hydraulic conductivity of the node into item 6b.

6b. [HY(NDSLAY)] – U1DREL.

   If IKVFLAG=0, NLAY > 1, and this is NOT the bottom layer, read item 7 for Vcont

7. [Vcont(NDSLAY)] – U1DREL. Note that Vcont read here is the interblock leakance between the node and a connected node below it. If there is no connecting node below, the Vcont value is ignored.

   If IKVFLAG=1 and NLAY > 1, then read item 8 for KV

8. [Kv(NDSLAY)] – U1DREL.

   Items 6 through 8 are read only for nodal input of conductivities (IKCFLAG=0).

9. [Sf2(NDSLAY)] – U1DREL If there is at least one transient stress period and

   LAYCON (see Ltype) of the layer is 2 or 3 or 4.

10. [WETDRY(NDSLAY)] – U1DREL If IWDFLG is not 0 and LAYCON of any layer is 1 or 3 (see Ltype).

   Items 11 through 15 are read only if Richards equation is solved by having the OPTION "RICHARDS" in the BAS file.

11. [ALPHA(NDSLAY)] – U1DREL

12. [BETA(NDSLAY)] – U1DREL

13. [SR(NDSLAY)] – U1DREL

14. [BROOK(NDSLAY)] – U1DREL

    Items 15 is read only if option BUBBLEPT is on when solving the Richards equation

15. [BP(NDSLAY)] – U1DREL

    Items 5 through 15 are read for unstructured input for each layer of the grid.

    If IKCFLAG = 1 or -1, indicating input of hydraulic conductivity (or transmissivity if confined) or inter-block conductance along connections, then read item 16 for all connections over all layers. Otherwise, Item 16 is not read.

16. [Ksat(NJA)] – U1DREL

    Otherwise, if UNSTRUCTURED option is not used then read items 17 through 28 for structured input

    A subset of the following two-dimensional variables is used to describe each layer. The variables needed for each layer depend on the layer-type code (LAYCON, which is defined as part of the Item-2 Ltype), whether the simulation has any transient stress periods (at least one stress period defined in the Discretization File specifies Ss/Tr as “TR”), and if the wetting capability is active (IWDFLG not 0). Unneeded variables must be omitted. In no situation will all variables be required. The required variables (Items 17-28) for layer 1 are read first; then the variables for layer 2 and so forth.

17. [Sf1(NCOL,NROW)] -- U2DREL If there is at least one transient stress period.

    If LAYCON is 0 or 2 (see Ltype), then read item 18.

18. [Tran(NCOL,NROW)] -- U2DREL.

    Otherwise, if LAYCON is 1 or 3 or 4 (see Ltype), read item 19.

19. [HY(NCOL,NROW)] -- U2DREL

If IKVFLAG is 0, then read item 19

20. [Vcont(NCOL,NROW)] -- U2DREL If not the bottom layer. Item 20 is omitted for the bottom-most layer or if there

Otherwise, if IKVFLAG is 1, then read item 21

21. [Kv(NCOL,NROW)] -- U2DREL

22. [Sf2(NCOL,NROW)] -- U2DREL If there is at least one transient stress period and

    LAYCON (see Ltype) is 2 or 3 or 4.

23. [WETDRY(NCOL,NROW)] -- U2DREL If IWDFLG is not 0 and LAYCON is 1 or 3 (see Ltype).

    Items 24 through 28 are input only if the Richards equation is solved by invoking the OPTION "RICHARDS" in the BAS file.

24. [ALPHA(NCOL,NROW)] -- U2DREL

25. [BETA(NCOL,NROW)] -- U2DREL

26. [SR(NCOL,NROW)] -- U2DREL

27. [BROOK(NCOL,NROW)] -- U2DREL

    Item 28 is read only if option BUBBLEPT is on when solving the Richards equation

28. [BP(NCOL,NROW)] -- U2DREL

    Items 17 through 28 are read for structured grid input only

Explanation of Variables Read by the BCF Package

IBCFCB—is a flag and a unit number.

If IBCFCB > 0, cell-by-cell flow terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control. The terms that are saved are storage, constant-head flow, and flow between adjacent cells.

If IBCFCB = 0, cell-by-cell flow terms will not be written.

If IBCFCB < 0, cell-by-cell flow for constant-head cells will be written in the listing file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control. Cell-by-cell flow to storage and between adjacent cells will not be written to any file.

HDRY—is the head that is assigned to cells that are converted to dry during a simulation. Although this value plays no role in the model calculations, HDRY values are useful as indicators when looking at the resulting heads that are output from the model. HDRY is thus similar to HNOFLO in the Basic Package, which is the value assigned to cells that are no-flow cells at the start of a model simulation.

IWDFLG—is a flag that determines if the wetting capability is active.

If IWDFLG = 0, the wetting capability is inactive.

If IWDFLG is not 0, the wetting capability is active

WETFCT—is a factor that is included in the calculation of the head that is initially established at a cell when that cell is converted from dry to wet. (See IHDWET.)

IWETIT—is the iteration interval for attempting to wet cells. Wetting is attempted every IWETIT iteration. This applies to outer iterations and not inner iterations. If IWETIT is 0, the value is changed to 1.

IHDWET—is a flag that determines which equation is used to define the initial head at cells that become wet:

If IHDWET = 0, equation 5-32A is used: h = BOT + WETFCT (hm - BOT) where is the head at the neighboring cell that causes cell n to convert to wet.

If IHDWET is not 0, equation 5-32B is used: h = BOT + WETFCT (THRESH)

IKVFLAG—is a flag indicating if vertical hydraulic conductivity is input instead of leakance between two layers.

If IKVFLAG = 0, the leakance between two layers is input as is standard for the BCF package.

If IKVFLAG is not 0, the vertical hydraulic conductivity of each layer is input and leakance is computed internally by the code as is done by the LPF package.

Note that the IKVFLAG should be zero for a model containing quasi 3D layers with input of leakance. Otherwise, the LPF package may be used.

IKCFLAG—is a flag indicating if hydraulic conductivity or transmissivity information is input for each of the nodes or whether this information is directly input for the nodal connections. The easiest input format is to provide the hydraulic conductivity or transmissivity values to the cells using a zero value for IKCFLAG.

If IKCFLAG = 0, the hydraulic conductivity or transmissivity values are input on a cell-by-cell basis with inter-block hydraulic conductivity or transmissivity value being computed as per the LAYAVG averaging scheme.

If IKCFLAG = 1, the hydraulic conductivity or transmissivity values are read for the connection between cells *n* and *m*.

If IKCFLAG = -1, the conductance values are read for the connection between cells *n* and *m*.

OPTIONS—are optional keywords that activate options:

BUBBLEPT indicates that, when the Richards equation is solved, the bubble point pressure head is also input. Without this option, it is assumed that air can enter the domain at the default pressure head of zero.

FULLYDRY indicates that, when the Richards equation is solved, the residual saturation is only applied to the relative permeability curve and soil saturation can vary from 0 to 1. Thus, soil saturation can be below residual saturation. In this case, the van Genuchten moisture retention function is applied with no residual saturation so the saturation can vary from 0 to 1. However, the relative permeability function uses an effective saturation that makes the relative permeability zero when saturation is at or below residual saturation causing flow to also be zero. Evapotranspiration or other local sink mechanisms can still remove water to be below the residual saturation value.

TABRICH nuzones nutabrows indicates that the Richards equation uses a tabular input for the moisture retention and relative permeability curves. The variable **nuzones** represents the number of soil types catalogued, and the variable **nutabrows** indicates the number of rows of tabular input for the moisture retention and relative permeability curves.

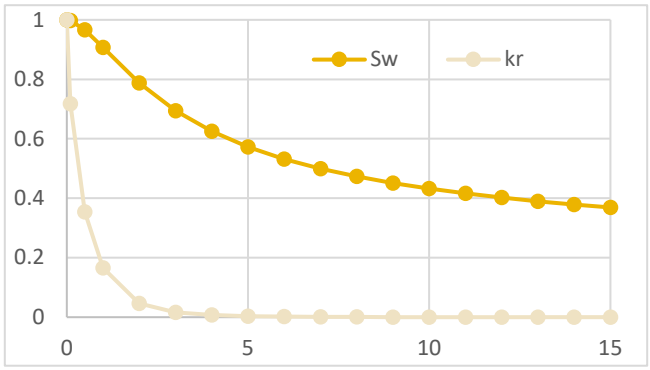
ALTSTO indicates that the alternate compressible (primary) storage formulation should be used for the simulation. The alternate formulation smoothly applies the storage coefficient from zero to full, over only a small distance from the top of a grid-block. This is the more conventional application of a storage coefficient but may be prone to greater numerical difficulties than the original formulation. No further input is required if this option is invoked.

IUZONTYP(NODES)—is an array containing the soil type index for all groundwater flow nodes. This array is read only for solving Richards Equation with tabular input of the moisture retention and relative permeability curves (i.e., LAYCON(K)=5 and TABRICH option is on). The index is used to identify the soil type from the catalogued tables of unsaturated zone properties. A value of zero may be entered for cells with a LAYCON(K) value other than 5.

RETCRVS(HC, SAT,Kr)—is a row within the table of moisture retention curve parameters for the various soils that are catalogued. The three items contained in the row are: HC, the capillary head; SAT, the saturation at that capillary head; and Kr, the relative permeability of the soil for that saturation and capillary head. This item is repeated "**nutabrows**" times for all the rows of a soil moisture retention table, which is then repeated "**nuzones**" times for each soil-type table in the catalogue. Note that the catalogue can contain more soil types than may be used through IUZONTYP in a simulation. The table should be ordered from low capillary pressure (zero at the water table) to high capillary pressure. An example table is shown below.

Hc	Sw	kr
0	1	1
0.1	0.9971	0.7176
0.5	0.966	0.3537
1	0.907	0.1652
2	0.788	0.0459
3	0.6945	0.0165
4	0.6251	0.0072
5	0.5727	0.0036
6	0.532	0.002

7	0.4995	0.0012
8	0.473	0.0008
9	0.4509	0.0005
10	0.4321	0.0004
11	0.416	0.0003
12	0.402	0.0002
13	0.3897	0.0001
14	0.3788	0.0001
15	0.3691	0.0001



Ltype—contains a combined code for each layer that specifies both the layer type (LAYCON) and the method of computing inter-block conductance. Use as many lines as needed to enter a value for each layer. Values are two-digit numbers:

The left digit defines the method of calculating inter-block transmissivity, LAYAVG. The methods are described by Goode and Appel (1992).

0 or blank—harmonic mean (the method used in MODFLOW-88).

1—arithmetic mean

2—logarithmic mean

3—arithmetic mean of saturated thickness and logarithmic-mean hydraulic conductivity.

The right digit defines the layer type (LAYCON), which is the same as in MODFLOW-88:

0—confined—Transmissivity and storage coefficient of the layer are constant for the entire simulation.

1—unconfined—Transmissivity of the layer varies and is calculated from the saturated thickness and hydraulic conductivity. The storage coefficient is constant. This type code is valid only for layer 1. Note that LAYCON = 1 should not be used when an IHM simulation is performed, and the layer 1 should use a value of 3 (or 4) instead, to indicate that it is convertible and could be confined or unconfined.

2—confined/unconfined—Transmissivity of the layer is constant. The storage coefficient may alternate between confined and unconfined values. Vertical flow from above is limited if the layer desaturates.

3—confined/unconfined—Transmissivity of the layer varies and is calculated from the saturated thickness and hydraulic conductivity. The storage coefficient may alternate between confined and unconfined values. Vertical flow from above is limited if the aquifer desaturates.

4—confined/unconfined—Unconfined transmissivity and convertible storage coefficient as in LAYCON of 3 above, however, the transmissivity is computed using upstream water table depth.

5—Unsaturated—Unsaturated flow solution is used for this layer. Note that a simulation can have some layers be unsaturated using Richards' Equation (where fine discretization may be required for accuracy), while other layers may solve for confined/unconfined flow using the LAYCON option 4 above (which provides accurate water table solutions with thick grid-blocks where soil moisture may not involve controlling processes or be a parameter of interest.

TRPY—is a one-dimensional variable containing a horizontal anisotropic factor for each layer and is the ratio of transmissivity or hydraulic conductivity (whichever is being used) along a column to transmissivity or hydraulic conductivity along a row. Set to 1.0 for isotropic conditions. This is a single variable with one value per layer. Do not read a variable for each layer—that is, include only one array control line for the entire variable.

ANGLEX—is the angle (in radians) between the horizontal x-axis and the outward normal to the face between a node and its connecting nodes (see figure 8 in documentation). The angle varies between zero and 6.283185 (two pi being 360 degrees). Also, the angle is needed only for evaluating anisotropy of a horizontal connection and the value that is entered for a vertical connection is ignored.

Sf1—is the primary storage coefficient. Read only if one or more transient stress periods are specified in the Discretization File. For LAYCON equal to 1, Sf1 will always be specific yield, whereas for LAYCON equal to 2 or 3, Sf1 will always be confined storage coefficient. For LAYCON equal to 0, Sf1 would normally be confined storage coefficient; however, a

LAYCON value of 0 also can be used to simulate water-table conditions where drawdowns everywhere are expected to remain a small fraction of the saturated thickness, and where there is no layer above, or flow from above is negligible. In this case, specific yield values would be entered for Sf1.

Tran—is the transmissivity along rows. Tran is multiplied by TRPY to obtain transmissivity along columns. For an unstructured grid, Tran is the transmissivity in the horizontal direction and TRPY is not input. Read only for layers where LAYCON is 0 or 2.

HY—is the hydraulic conductivity along rows. HY is multiplied by TRPY to obtain hydraulic conductivity along columns. For an unstructured grid, HY is the hydraulic conductivity in the horizontal direction and TRPY is not input. Read only for layers where LAYCON is 1 or 3 or 4.

Vcont—is the vertical hydraulic conductivity divided by the thickness from a layer to the layer below (also called leakance). The value for a cell is the hydraulic conductivity divided by thickness for the material between the node in that cell and the node in the cell below. Because there is not a layer beneath the bottom layer, Vcont cannot be specified for the bottom layer. If unstructured grids are used, Vcont is read for every node, however, the value is ignored when a node does not have corresponding node in an underlying layer.

Kv—is the vertical hydraulic conductivity of the cell and the leakance is computed for each vertical connection.

Sf2—is the secondary storage coefficient. Read only for layers where LAYCON is 2 or 3 and only if there are one or more transient stress periods specified in the Discretization File. The secondary storage coefficient is always specific yield.

WETDRY—is a combination of the wetting threshold (THRESH) and a flag to indicate which neighboring cells can cause a cell to become wet. If WETDRY < 0, only the cells below a dry cell can cause the cell to become wet. If WETDRY > 0, then any of the adjacent connected cells can cause a cell to become wet. If WETDRY is 0, the cell cannot be wetted. The absolute value of WETDRY is the wetting threshold. When the sum of BOT and the absolute value of WETDRY at a dry cell is equaled or exceeded by the head at an adjacent cell, the cell is wetted. Read only if LAYCON is 1 or 3 and IWDFLG is not 0. Note that

WETDRY is read for every node in the grid if LAYCON of any layer is 1 or 3. For layers where LAYCON is not 1 or 3, the value is ignored.

ALPHA—is the van Genuchten alpha parameter for moisture retention.

BETA—is the van Genuchten beta parameter for moisture retention.

SR—is the van Genuchten SR parameter for moisture retention.

BROOK—is the Brooks-Corey exponent for relative permeability. ***Note that if a negative value is supplied for this parameter for any cell, the van Genuchten relative permeability curve is used for that cell (as the upstream cell) when computing the relative permeability instead of the Brooks-Corey relative permeability function.***

BP—is the bubbling point pressure head below which gas is produced.

Ksat—is the inter-block saturated hydraulic conductivity or transmissivity (if IKCFLAG = 1) or the inter-block conductance (if IKCFLAG = - 1) of the connection between nodes *n* and *m*. This is the most general form of input of hydraulic flow properties and includes the impact of anisotropy in any direction, hydraulic flow barriers or confining layers between nodes. For IKCFLAG = 1, if LAYCON is 0 or 2 for a layer, then Ksat is the transmissivity for a horizontal direction connection and the saturated vertical hydraulic conductivity for a vertical direction connection. For IKCFLAG = 1, if LAYCON is 4 for a layer, then Ksat is the saturated hydraulic conductivity for a horizontal direction connection and the saturated vertical hydraulic conductivity for a vertical direction connection. LAYCON cannot be 1 or 3 with IKCFLAG=1 because individual cell hydraulic conductivities are required for transmissivity computations with LAYTYP=1, which are not available when IKCFLAG=1 If IKCFLAG=-1, the inter-block conductance of the connected cells is input.

LAYER-PROPERTY FLOW (LPF) PACKAGE INPUT WITH UNSATURATED FLOW

Input for the Layer-Property Flow (LPF) Package is read from the file that is type "LPF" in the Name File. Free format is used for reading all values. The LPF Package is an alternative to the BCF Package. The two packages should not be used simultaneously.

Options in addition to MODFLOW-USG capabilities include:

- Option to compute compressible storage with an alternate formulation (ALTSTO). Instead of compressible storage changing from zero to full with grid block saturation, it is smoothly applied over only a small distance from the top of a grid-block. This is the more conventional application of a storage coefficient but may have more numerical difficulties than the original formulation. No further input is required when using this option aside from calling it out in the "options" section.

- Solution of 3-dimensional Richards' Equation for unsaturated zone domain. This option can be invoked in the BAS file for the whole domain or can be applied here on a layer-by-layer basis. For instance, the top few layers of a model may be simulated as "unsaturated", with the remaining layers below being "unconfined". Text in this color may be skipped if Richards' equation is not solved by the model.

FOR EACH SIMULATION

0. [#Txt]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

If *UNSTRUCTURED* option is used, then read item 1a

1a. ILPFCB HDRY NPLPF IKCFLAG [Options]

Otherwise, if *UNSTRUCTURED* option is not used, then read item 1b for structured input

1b. ILPFCB HDRY NPLPF [Options]

Read items 1c and 1d below, only if the TABRICH option is invoked above, to indicate tabular input of moisture retention and relative permeability curves.

1c. IUZONTAB(NODES) -- U1DINT

1d. RETCRVS(HC, SAT,Kr)

Item 1d is the tabular input of moisture retention parameters of each soil type and is repeated "**nutabrows**" times for all the rows of the table, which is then repeated "**nuzones**" times for each soil type in the catalogue.

2. LAYTYP(NLAY)
3. LAYAVG(NLAY)
4. CHANI(NLAY)
5. LAYVKA(NLAY)
6. LAYWET(NLAY)
7. [WETFCT IWETIT IHDWET]

   (Include item 7 only if LAYWET indicates at least one wettable layer.)

8. [PARNAM PARTYP Parval NCLU]
9. [Layer Mltarr Zonarr IZ]

   Each repetition of Item 9 is called a parameter cluster. Repeat Item 9 NCLU times.

   Repeat Items 8-9 for each parameter to be defined (that is, NPLPF times).

   A subset of the following two-dimensional variables is used to describe each layer. All the variables that apply to layer 1 are read first, followed by layer 2, followed by layer 3, and so forth. A variable not required due to simulation options (for example, Ss and Sy for a completely steady-state simulation) must be omitted from the input file. Also note that there may be different numbers of nodes per layer (NDSLAY) for an unstructured grid.

   These variables are either read by the array-reading utility subroutine, U2DREL for a structured grid or U1DREL for an unstructured grid, or they are defined through parameters. If a variable is defined through parameters, then the variable itself is not read; however, a single line containing a print code is read in place of the control line. The print code determines the format for printing the values of the variable as defined by parameters. The print codes are the same as those used in a control line. If any parameters of a given type are used, parameters must be used to define the corresponding variable for all layers in the model.

If UNSTRUCTURED option is used, then read item 10 if IKCFLAG=0 for nodal input of the conductivity parameters and there is anisotropy in the system (that is, any of CHANI is not equal to one).

10. [ANGLEX(NJAG)] – U1DREL.

If *UNSTRUCTURED* option is used then read items 11 through 22. Items 11 through 21 are read layer by layer and item 22 (if needed) is read for the entire grid after items 11 through 21 are read (where needed) for all layers in the grid.

If *IKCFLAG=0* for nodal input of conductivities, then read items 11, 12 and 13 otherwise skip these data items.

11. HK(NDSLAY) If any HK parameters are included, read only a print code.

12. [HANI(NDSLAY)] Include item 12 only if CHANI is less than or equal to 0. If any HANI parameters are included, read only a print code.

13. VKA(NDSLAY) If any VK or VANI parameters are included, read only a print code.

    Items 11, 12 and 13 are read only for nodal input of hydraulic conductivities (*IKCFLAG=0*).

14. [Ss(NDSLAY)] Include item 14 only if at least one stress period is transient. If there are any SS parameters, read only a print code.

15. [Sy(NDSLAY)] Include item 15 only if at least one stress period is transient and LAYTYP is not 0. If any SY parameters are included, read only a print code.

16. [VKCB(NDSLAY)] Include item 16 only if IKCFLAG=0 and LAYCBD (in the Discretization File) is not 0. If any VKCB parameters are included, read only a print code.

17. [WETDRY(NDSLAY)] Include item 17 only if LAYWET is not 0 and LAYTYP is not 0 or 4.

    Items 18 through 21 are read only if Richards equation is solved by having the OPTION "RICHARDS" in the BAS file.

18. [ALPHA(NDSLAY)] – U1DREL

19. [BETA(NDSLAY)] – U1DREL

20. [SR(NDSLAY)] – U1DREL

21. [BROOK(NDSLAY)] – U1DREL

    Items 22 is read only if option BUBBLEPT is on when solving the Richards equation.

22. [BP(NDSLAY)] – U1DREL

    If IKCFLAG = 1 or -1, indicating input of hydraulic conductivity (or transmissivity if confined) or inter-block conductance along connections then read item 23 for all connections over all layers. Otherwise, Item 23 is not read.

23. [Ksat(NJA)] – U1DREL

    Otherwise, if *UNSTRUCTURED* option is not used, then read items 24 through 35 for structured input. Items 24 through 35 are read layer by layer.

24. HK(NCOL,NROW) If any HK parameters are included, read only a print code.

25. [HANI(NCOL,NROW)] Include item 25 only if CHANI is less than or equal to 0. If any HANI parameters are included, read only a print code.

26. VKA(NCOL,NROW) If any VK or VANI parameters are included, read only a print code.

27. [Ss(NCOL,NROW)] Include item 27 only if at least one stress period is transient. If there are any SS parameters, read only a print code.

28. [Sy(NCOL,NROW)] Include item 28 only if at least one stress period is transient and LAYTYP is not 0. If any SY parameters are included, read only a print code.

29. [VKCB(NCOL,NROW)] Include item 29 only if LAYCBD (in the Discretization File) is not 0. If any VKCB parameters are included, read only a print code.

30. [WETDRY(NCOL,NROW)] Include item 30 only if LAYWET is not 0 and LAYTYP is not 0.

    Items 31 through 35 are input only if the Richards equation is solved by invoking the OPTION “RICHARDS” in the BAS file.

31. [ALPHA(NCOL,NROW)] -- U2DREL

32. [BETA(NCOL,NROW)] -- U2DREL

33. [SR(NCOL,NROW)] -- U2DREL

34. [BROOK(NCOL,NROW)] -- U2DREL

    Items 35 is read only if option BUBBLEPT is on when solving the Richards equation

35. [BP(NCOL,NROW)] -- U2DREL

Explanation of Variables Read by the LPF Package

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

ILPFCB—is a flag and a unit number.

If ILPFCB > 0, cell-by-cell flow terms will be written to this unit number when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control. The terms that are saved are storage, constant-head flow, and flow between adjacent cells.

If ILPFCB = 0, cell-by-cell flow terms will not be written.

If ILPFCB < 0, cell-by-cell flow for constant-head cells will be written in the listing file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control. Cell-by-cell flow to storage and between adjacent cells will not be written to any file.

HDRY—is the head that is assigned to cells that are converted to dry during a simulation. Although this value plays no role in the model calculations, HDRY values are useful as indicators when looking at the resulting heads that are output from the model. HDRY is thus similar to HNOFLO in the Basic Package, which is the value assigned to cells that are no-flow cells at the start of a model simulation.

NPLPF—is the number of LPF parameters.

IKCFLAG—is a flag indicating if hydraulic conductivity or transmissivity information is input for each of the cells or whether this information is directly input for the nodal connections.

If IKCFLAG =0, the hydraulic conductivity or transmissivity values are input on a cell-by-cell basis with inter-block hydraulic conductivity or transmissivity value being computed as per the LAYAVG averaging scheme.

If IKCFLAG = 1, the hydraulic conductivity or transmissivity values are read for the connection between cells *n* and *m*.

If IKCFLAG = -1, the conductance values are read for the connection between cells *n* and *m*.

OPTIONS—are optional keywords that activate options:

STORAGECOEFFICIENT indicates that variable Ss and SS parameters are read as storage coefficient rather than specific storage.

CONSTANTCV indicates that vertical conductance for an unconfined cell is computed from the cell thickness rather than the saturated thickness.

THICKSTRT indicates that layers having a negative LAYTYP are confined, and their cell thickness for conductance calculations will be computed as STRT-BOT rather than TOP-BOT.

NOCVCORRECTION indicates that vertical conductance is not corrected when the vertical flow correction is applied.

NOVFC indicates that the vertical flow correction under dewatered conditions (described on p. 5-8 of USGS Techniques and Methods Report 6-A16) is turned off. Also, the vertical conduction correction described on p. 5-18 of that report is turned off.

NOPARCHECK indicates that, when parameters define an array, there is no check to see if a value is defined for all cells. The value is 0 at cells for which parameters do not define a value. If this option is not specified, the simulation aborts if a value is not defined for all cells.

ALTSTO indicates that the alternate compressible (primary) storage formulation should be used for the simulation. The alternate formulation smoothly applies the storage coefficient from zero to full, over only a small distance from the top of a grid-block. This is the more

conventional application of a storage coefficient but may be prone to greater numerical difficulties than the original formulation. No further input is required if this option is selected.

BUBBLEPT indicates that, when the Richards equation is solved, the bubble point pressure head is also input. Without this option, it is assumed that air can enter the domain at the default pressure head of zero.

FULLYDRY indicates that, when the Richards equation is solved, the residual saturation is only applied to the relative permeability curve and soil saturation can vary from 0 to 1. Thus, soil saturation can be below residual saturation. In this case, the van Genuchten moisture retention function is applied with no residual saturation so the saturation can vary from 0 to 1. However, the relative permeability function uses an effective saturation that makes the relative permeability zero when saturation is at or below residual saturation causing flow to also be zero. Evapotranspiration or other local sink mechanisms can still remove water to be below the residual saturation value.

TABRICH nuzones nutabrows indicates that the Richards equation uses a tabular input for the moisture retention and relative permeability curves. The variable **nuzones** represents the number of soil types catalogued, and the variable **nutabrows** indicates the number of rows of tabular input for the moisture retention and relative permeability curves.

IUZONTYP(NODES)—is an array containing the soil type index for all groundwater flow nodes. This array is read only for solving Richards Equation with tabular input of the moisture retention and relative permeability curves (i.e., LAYCON(K)=5 and TABRICH option is on). The index is used to identify the soil type from the catalogued tables of unsaturated zone properties. A value of zero may be entered for cells with a LAYCON(K) value other than 5.

RETCRVS(HC, SAT,Kr)—is a row within the table of moisture retention curve parameters for the various soils that are catalogued. The three items contained in the row are: HC, the capillary head; SAT, the saturation at that capillary head; and Kr, the relative permeability of the soil for that saturation and capillary head. This item is repeated "**nutabrows**" times for all the rows of a soil moisture retention table, which is then repeated "**nuzones**" times for each soil-type table in the catalogue. Note that the catalogue can contain more soil types than may be used through IUZONTYP in a simulation.

LAYTYP—contains a flag for each layer that specifies the layer type.

0 – confined

>0 – convertible

= 4 – convertible, with transmissivity computed using upstream weighting formulation

= 5 – unsaturated flow simulation. Unsaturated flow solution is used for this layer. Note that a simulation can have some layers be unsaturated using Richards' Equation (where fine discretization may be required for accuracy), while other layers may solve for confined/unconfined flow using the LAYCON option 4 above (which provides accurate water table solutions with thick grid-blocks where soil moisture may not involve controlling processes or be a parameter of interest.

<0 – convertible unless the THICKSTRT option is in effect. When THICKSTRT is in effect, a negative value of LAYTYP indicates that the layer is confined, and its saturated thickness will be computed as STRT-BOT.

LAYAVG—contains a flag for each layer that defines the method of calculating interblock transmissivity.

0—harmonic mean

1— logarithmic mean

2— arithmetic mean of saturated thickness and logarithmic-mean hydraulic conductivity

CHANI—contains a value for each layer that is a flag or the horizontal anisotropy. If CHANI is less than or equal to 0, then variable HANI defines horizontal anisotropy. If CHANI is greater than 0, then CHANI is the horizontal anisotropy for the entire layer, and HANI is not read. If any HANI parameters are used, CHANI for all layers must be less than or equal to 0.

LAYVKA—contains a flag for each layer that indicates whether variable VKA is vertical hydraulic conductivity or the ratio of horizontal to vertical hydraulic conductivity.

0—indicates VKA is vertical hydraulic conductivity

not 0—indicates VKA is the ratio of horizontal to vertical hydraulic conductivity, where the horizontal hydraulic conductivity is specified as HK in item 10.

LAYWET—contains a flag for each layer that indicates whether wetting is active.

0—indicates wetting is inactive

not 0—indicates wetting is active

WETFCT—is a factor that is included in the calculation of the head that is initially established at a cell when the cell is converted from dry to wet. (See IHDWET.)

IWETIT—is the iteration interval for attempting to wet cells. Wetting is attempted every IWETIT iteration. If using the PCG solver (Hill, 1990), this applies to outer iterations, not inner iterations. If IWETIT ≤ 0, the value is changed to 1.

IHDWET—is a flag that determines which equation is used to define the initial head at cells that become wet:

If IHDWET = 0, equation 5-32A in Harbaugh (2005) is used: h = BOT + WETFCT (hn - BOT) .

If IHDWET is not 0, equation 5-32B in Harbaugh (2005) is used: h = BOT + WETFCT(THRESH) .

PARNAM—is the name of a parameter to be defined. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter to be defined. For the LPF Package, the allowed parameter types are:

HK—defines variable HK, horizontal hydraulic conductivity

HANI—defines variable HANI, horizontal anisotropy

VK—defines variable VKA for layers for which VKA represents vertical hydraulic conductivity (LAYVKA=0)

VANI—defines variable VKA for layers for which VKA represents vertical anisotropy (LAYVKA≠0)

SS—defines variable Ss, the specific storage

SY—defines variable Sy, the specific yield

VKCB—defines variable VKCB, the vertical hydraulic conductivity of a Quasi-3D confining layer.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NCLU—is the number of clusters required to define the parameter. Each repetition of Item 9 is a cluster (variables Layer, Mltarr, Zonarr, and IZ). Each layer that is associated with a parameter usually has only one cluster. For example, parameters which apply to cells in a single layer generally will be defined by just one cluster. However, having more than one cluster for the same layer is acceptable.

Layer—is the layer number to which a cluster definition applies.

Mltarr—is the name of the multiplier array to be used to define variable values that are associated with a parameter. The name "NONE" means that there is no multiplier array, and the variable values will be set equal to Parval.

Zonarr—is the name of the zone array to be used to define the cells that are associated with a parameter. The name "ALL" means that there is no zone array, and all cells in the specified layer are part of the parameter.

IZ—is up to 10 zone numbers (separated by spaces) that define the cells that are associated with a parameter. These values are not used if ZONARR is specified as "ALL". Values can be positive or negative, but 0 is not allowed. The end of the line, a zero value, or a non-numeric entry terminates the list of values.

ANGLEX—is the angle (in radians) between the horizontal x-axis and the outward normal to the face between a node and its connecting nodes (see figure 8 in MODFLOW-USG report). The angle varies between zero and 6.283185 (two pi being 360 degrees). Also, the angle is needed only for evaluating anisotropy of a horizontal connection and the value that is entered for a vertical connection is ignored.

HK—is the hydraulic conductivity along rows. HK is multiplied by horizontal anisotropy (see CHANI and HANI) to obtain hydraulic conductivity along columns.

HANI—is the ratio of hydraulic conductivity along columns to hydraulic conductivity along rows, where HK of item 10 specifies the hydraulic conductivity along rows. Thus, the hydraulic conductivity along columns is the product of the values in HK and HANI. Read only if CHANI ≤ 0.

VKA—is either vertical hydraulic conductivity or the ratio of horizontal to vertical hydraulic conductivity depending on the value of LAYVKA. If LAYVKA is 0, VKA is vertical hydraulic conductivity. If LAYVKA is not 0, VKA is the ratio of horizontal to vertical hydraulic conductivity. In this case, HK is divided by VKA to obtain vertical hydraulic conductivity, and values of VKA typically are greater than or equal to 1.0.

Ss—is specific storage unless the STORAGECOEFFICIENT option is used. When STORAGECOEFFICIENT is used, Ss is confined storage coefficient. Read only for a transient simulation (at least one transient stress period).

Sy—is specific yield. Read only for a transient simulation (at least one transient stress period) and if the layer is convertible (LAYTYP is not 0).

VKCB—is the vertical hydraulic conductivity of a quasi-three-dimensional confining bed below a layer. Read only if there is a confining bed. Because the bottom layer cannot have a confining bed, VKCB cannot be specified for the bottom layer.

WETDRY—is a combination of the wetting threshold and a flag to indicate which neighboring cells can cause a cell to become wet. If WETDRY < 0, only the cell below a dry cell can cause the cell to become wet. If WETDRY > 0, the cell below a dry cell and the four horizontally adjacent cells can cause a cell to become wet. If WETDRY is 0, the cell cannot be wetted. The absolute value of WETDRY is the wetting threshold. When the sum of BOT and the absolute value of WETDRY at a dry cell is equaled or exceeded by the head at an adjacent cell, the cell is wetted. Read only if LAYTYP is not 0 and LAYWET is not 0. Note that WETDRY is read for every node in the grid if LAYCON of any layer is 1 or 3. For layers where LAYCON is not 1 or 3, the value is ignored.

ALPHA—is the van Genuchten alpha parameter for moisture retention.

BETA—is the van Genuchten beta parameter for moisture retention.

SR—is the van Genuchten SR parameter for moisture retention.

BROOK—is the Brooks-Corey exponent for relative permeability. ***Note that if a negative value is supplied for this parameter for any cell, the van Genuchten relative permeability curve is used for that cell (as the upstream cell) when computing the relative permeability instead of the Brooks-Corey relative permeability function.***

BP—is the bubbling point pressure head below which gas is produced.

Ksat—is the inter-block saturated hydraulic conductivity or transmissivity (if IKCFLAG = 1) or the inter-block saturated conductance (if IKCFLAG = - 1) of the connection between nodes *n* and *m*. This is the most general form of input of hydraulic flow properties and includes the impact of anisotropy in any direction, hydraulic flow barriers or confining layers between nodes. For IKCFLAG = 1, if LAYTYP is 0 for a layer, then Ksat is the transmissivity for a horizontal direction connection and the saturated vertical hydraulic conductivity for a vertical direction connection. For IKCFLAG = 1, if LAYTYP is 4 for a layer, then Ksat is the saturated hydraulic conductivity for a horizontal direction connection and the saturated vertical hydraulic conductivity for a vertical direction connection. LAYTYP cannot be 1 with IKCFLAG=1 because individual cell hydraulic conductivities are required for transmissivity computations with LAYTYP=1, which are not available when IKCFLAG=1. If IKCFLAG=-1, the inter-block conductance of the connected cells is input. Note that the variable CHANI is ignored if Ksat is read to provide the inter-block flow variable.

HYDRAULIC FLOW BARRIER (HFB6) PACKAGE INPUT

The Horizontal Flow Barrier Package of MODFLOW-2005 is renamed the Hydraulic Flow Barrier Package with the same abbreviation HFB. This is because the functionality of the hydraulic flow barrier is the same as that of the horizontal flow barrier, however, it may also be applied in the vertical direction as a quasi-3D confining layer, simply by allowing the two nodes between which the barrier is placed, to be vertically connected.

The HFB can be made transient if the TRANSIENT option is used in the HFB input file. This allows for changing the HFB properties at every stress period. If the HFB is transient then the value can be changed at every stress period. If a HFN does not exist during a portion of the simulation (for example if the HFB represents a reactive flow barrier which is emplaced only in

some later stress period), then its leakance (hydraulic conductivity divided by thickness of the barrier) can be given a high value. Note that too high a value can cause convergence issues therefore using the hydraulic conductivity of the soil as the leakance (assuming unit thickness) is a reasonable approach.

Input for the Hydraulic Flow Barrier (HFB) Package is read from the file that has file type "HFB6" in the Name File. All variables are read in free format. Note that the HFB package only applies to the Groundwater Flow Process.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1a. NPHFB MXFB NHFBNP [OPTIONS]

Item 1b below is read only if the TRANSIENT_HFB option is read as an options keyword

1b. IHFBRD

2. [PARNAM PARTYP Parval NLST]

If UNSTRUCTURED option is used then read item 3a

3a. [Node1 Node2 Factor]

These variables are free format.

Otherwise, if UNSTRUCTURED option is not used then read item 3b for structured input

3b. [Layer IROW1 ICOL1 IROW2 ICOL2 Factor]

Repeat Items 2 and 3 NPHFB times. Items 2 and 3 are not read if NPHFB is negative or zero.

NLST repetitions of Item 3 are required; they are read by subroutine ULSTRD. (SFAC of the ULSTRD utility subroutine applies to Factor).

If UNSTRUCTURED option is used then read item 4a

4a. Node1 Node2 Hydchr

These variables are free format.

Otherwise, if UNSTRUCTURED option is not used then read item 4b for structured input

4b. Layer IROW1 ICOL1 IROW2 ICOL2 Hydchr

NHFBNP repetitions of Item 4 are read. Item 4 is not read if NHFBNP is negative or zero.

5. NACTHFB

6. Pname

NACTHFB repetitions of Item 6 are read. Item 6 is not read if NACTHFB is negative or zero.

Explanation of Variables Read by the HFB Package:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPHFB—is the number of horizontal flow barrier parameters to be defined in Items 2 and 3. Note: An HFB parameter must be defined in Items 2 and 3, and made active using Item 6, to have an effect in the simulation.

MXFB—is the maximum number of HFB barriers that will be defined using parameters.

NHFBNP—is the number of HFB barriers not defined by parameters.

OPTIONS are keyword options. "OPTIONS" must be listed as the first keyword in order to specify any options. The following options are supported:

TRANSIENT_HFB indicates that transient HFB information will be read for each stress period. ***Note that the number and location of the HFBs should not vary between stress periods, only the leakance value of the HFB should be changed.***

NOPRINT will suppress printout of the list of flow barriers provided in the HFB input file.

IHFBRD—is an index and a flag indicating if the HFB values are to be read at the current stress period. This flag is read only if the TRANSIENT_HFB option is selected.

If IHFBRD = -1 or 0 then use the HFBs from the previous stress period

If IHFBRD > 0 then read HFB values for the current stress period. Note that IHFBRD should be set greater than zero for the first stress period so that the information can be read.

PARNAM—is the name of a parameter. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter. For the HFB Package, the only allowed parameter type is HFB, which defines values of the hydraulic characteristic of the barrier.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NLST—is the number of horizontal flow barrier cells included in the parameter.

Layer—is the number of the model layer in which the horizontal flow barrier is located.

IROW1—is the row number of the cell on one side of the horizontal flow barrier.

ICOL1—is the column number of the cell on one side of the horizontal flow barrier.

I**ROW2**—is the row number of the cell on the other side of the horizontal flow barrier.

ICOL2—is the column number of the cell on the other side of the horizontal flow barrier.

Node1—is the node number of the cell on one side of the horizontal flow barrier. Note that the HFB is applied only between two nodes of the GWF Process domain.

Node2—is the node number of the cell on the other side of the horizontal flow barrier. Note that the HFB is applied only between two nodes of the GWF Process domain.

Factor—is the factor used to calculate hydraulic characteristic from the parameter value. The hydraulic characteristic is the product of Factor and the parameter value.

Hydchr—is the hydraulic characteristic of the horizontal flow barrier. The hydraulic characteristic is the barrier hydraulic conductivity divided by the width of the horizontal flow barrier.

NACTHFB—is the number of active HFB parameters.

Pname—is the name of a parameter to be used in the simulation. NACTHFB parameter names will be read.

DUAL POROSITY FLOW (DPF) PACKAGE INPUT

Input for the Dual Porosity Flow (DPF) Package is read from the file that has file type "DPF" in the Name File. All variables are read in free format. Note that the DPF package only applies for the Groundwater Flow Process. Note that this input is read only in an unstructured format, even if the structured format option is selected. However, output of heads and cell-by-cell fluxes will be in a structured format, if the structured option is selected. The input provided in the DPF package is for the immobile domain (matrix domain) while the mobile domain (fracture domain) input is provided in the BCF or LPF input file. The immobile domain uses the same aquifer type as the mobile domain provided in the BCF or LPF file. Thus, if a cell is represented by Richards' Equation in the BCT or LPF file, then the same cell will also be represented by Richards' Equation in the immobile domain here.

FOR EACH SIMULATION

0. [#Text]

   Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. IDPFCB IDPFHD IDPFDD

   Item 2 is read for layer 1 first; then for layer 2 and so forth. Note that there may be a different number of nodes specified for each layer (NDSLAY) for an unstructured grid.

Read item 1B below, only if the TABRICH option is invoked in the BCF/LPF files, to indicate tabular input of moisture retention and relative permeability curves.

1B. IUZONTABIM(NODES) -- U1DINT

2. IBOUNDIM(NDSLAY) – U1DINT

   Item 3 is read for layer 1 first; then for layer 2 and so forth. Note that there may be a different number of nodes specified for each layer (NDSLAY) for an unstructured grid.

3. HNEWIM(NDSLAY) – U1DREL

   A subset of the following one-dimensional variables is used to describe each node. The variables needed for each node depend on the layer-type code of the layer in which the node resides (LAYCON, which is defined as part of the Item-2 Ltype), whether the simulation has any transient stress periods (at least one stress period defined in the Discretization File specifies Ss/Tr as "TR"), and if Richards equation is solved or not. Unneeded variables must be omitted. All variables may not be required.

   The required variables for Items 4-10 for layer 1 are read first; then the variables for layer 2 and so forth. Also note that there may be different number of nodes per layer (NDSLAY) for an unstructured grid.

4. [PHIF(NDSLAY)] – U1DREL

5. [DDFTR(NDSLAY)] – U1DREL

6. [SC1IM(NDSLAY)] – U1DREL

   Item 7 is read only if the flow simulation is unconfined for this layer.

7. [SC2IM(NDSLAY)] – U1DREL

   Items 8-12 are read only if the flow simulation is for Richards equation, and they are only read for layers that solve for Richards equation, if other layers are solving for confined or unconfined flow.

8. [ALPHAIM(NDSLAY)] – U1DREL

9. [BETAIM(NDSLAY)] – U1DREL

10. [SRIM(NDSLAY)] – U1DREL

11. [BROOKIM(NDSLAY)] – U1DREL

    Items 12 is read only if the option BUBBLEPT is turned on in the BCF or LPF package input.

12. [BPIM(NDSLAY)] – U1DREL

Explanation of Variables Read by the DPF Package

IDPFCB—is a flag and a unit number.

If IDPFCB > 0, cell-by-cell flow terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control. The terms that are saved are storage, constant-head flow, and flow between adjacent cells.

If IDPFCB = 0, cell-by-cell flow terms will not be written.

If IDPFCB < 0, cell-by-cell flow for constant-head cells will be written in the listing file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control. Cell-by-cell flow to storage and between adjacent cells will not be written to any file.

IDPFHD—is a flag and a unit number.

If IDPFHD > 0, immobile domain heads will be written to this unit number in a binary format when "SAVE HEAD" or a nonzero value for IHDSV is specified in Output Control.

If IDPFHD = 0, immobile domain heads will not be saved.

If IDPFHD < 0, immobile domain heads will be written to the listing file.

IDPFDD—is a flag and a unit number.

If IDPFDD > 0, immobile domain drawdown (or saturation if Richards equation is solved) will be written to this unit number in a binary format when "SAVE DRAWDOWN" or a nonzero value for IDDSV is specified in Output Control.

If IDPFDD = 0, immobile domain drawdown will not be saved.

If IDPFDD < 0, immobile domain drawdown will be written to the listing file.

IUZONTYPIM(NODES)—is an array containing the soil type index for all groundwater flow nodes in the immobile domain. This array is read only for solving Richards Equation with tabular input of the moisture retention and relative permeability curves (i.e., LAYCON(K)=5 and TABRICH option is on in the BCF/LPF file). The index is used to identify the soil type from the catalogued tables of unsaturated zone properties. A value of zero may be entered

for cells with a LAYCON(K) value other than 5. The catalogue of soil types and their moisture retention properties is maintained in the BCF/LPF file.

IBOUNDIM—is the boundary variable for the immobile domain. One value is read for every model cell. Usually, these values are read one layer at a time; however, when the XSECTION option is specified, a single two-dimensional variable for the cross section is read.

If IBOUNDIM < 0, cell J,I,K has a constant head.

If IBOUNDIM = 0, cell J,I,K is no flow.

HNEWIM—is initial (starting) head in the immobile domain—that is, head at the beginning of the simulation. HNEWIM must be specified for all simulations, including steady-state simulations. One value is read for every model cell. Usually, these values are read a layer at a time. When the XSECTION option is specified, however, a single two-dimensional variable for the cross section is read.

PHIF—is the mobile fraction. i.e., the fraction of the total space that contains the mobile domain.

DDFTR—is the dual domain flow transfer rate.

SC1IM—is the specific storage of the immobile domain.

SC2IM—is the specific yield or porosity of the immobile domain.

ALPHAIM—is the van Genuchten alpha coefficient of the immobile domain.

BETAIM—is the van Genuchten beta coefficient of the immobile domain.

SRIM—is the van Genuchten sr coefficient of the immobile domain.

BROOKIM—is the Brooks-Corey exponent for the relative permeability of the immobile domain.

Note that if a negative value is supplied for this parameter for any cell, the van Genuchten relative permeability curve is used for that cell (as the upstream cell) when computing the relative permeability instead of the Brooks-Corey relative permeability function.

BPIM—is the bubble point or air entry pressure head of the immobile domain.

CONNECTED LINEAR NETWORK (CLN) PROCESS INPUT INSTRUCTIONS WITH TURBULENT FLOW, WELL EFFICIENCY AND TRANSPORT

Input for the Connected Linear Network (CLN) Process is read from the file that is type "CLN" in the Name File. Options have been used to expand the capability of MODFLOW-USG, to keep the code backward compatible. An additional optional input of the coordinates of a CLN segment is also included. These coordinates are not used by the code but provide the beginning and ending location of each segment in 3-D cartesian coordinates which enables placing them in space for use with plotting and Graphic User Interfaces.

The CLN process input also handles input for transport related parameters. Special options are provided for heat transport simulations to simulate Borehole Heat Exchangers (BHEs) using CLN tubes. Specifically, the BHEs may include resistance to heat transfer between GWF and CLN domain. Also, the BHE fluid may be different from water in the GWF domain. Finally, a convective heat coefficient for the BHEs may be included in the heat conductance equation. These input for BHEs are invoked when BHEDETAIL option is used under OPTIONS2 in item 1 of data input indicated below.

FOR EACH SIMULATION

0. [OPTIONS opt, …]

This optional item must start with the keyword "OPTIONS"

1. **NCLN ICLNNDS ICLNCB ICLNHD ICLNDD ICLNIB NCLNGWC NCONDUITYP [OPTIONS2]**

   These variables are free format if the option "FREE" is specified in the Basic Package input file; otherwise, the variables all have 10-character fields.

   If NCLN is greater than zero, then read item 2.

2. **NNDCLN(NCLN) – U1DREL**

   If NCLN is greater than zero and ICLNNDS is greater than zero, then read item 3. Item 3 is read NCLN times, once for each CLN segment in the simulation. The number of entries for

each line of item 3 is the number of CLN cells (NNDCLN) associated with each CLN segment, as input in item 2 above.

3. **CLNCON[NNDCLN(NCLN)]**
   The variables of item 3 are free format if the option "FREE" is specified in the Basic Package input file; otherwise, the variables all have 10-character fields.

   If NCLN is equal to zero, then read items 4, 5, and 6.

4. **NJA_CLN**

5. **IAC_CLN(NODES) - U1DINT**

6. **JA_CLN(NJAG) - U1DINT**

7. **IFNO IFTYP IFDIR FLENG FELEV FANGLE IFLIN ICCWADI [X1 Y1 Z1 X2 Y2 Z2]**
   Item 7 is read for each CLN node in the domain. Therefore, item 7 is repeated NCLNNDS times for each of the NCLNNDS Connected Linear Network nodes. The last 6 items in brackets are the coordinates of a CLN cell and help to draw that cell in space for graphics and GUIs.

If UNSTRUCTURED option is used then read item 8.

8. **IFNOD IGWNOD IFCON FSKIN FLENGW FANISO ICGWADI**
   Item 8 is read for each CLN node to porous medium grid-block connection in the domain. Therefore, item 8 is repeated NCLNGWC times for each of the NCLNGWC connections.

Otherwise, if UNSTRUCTURED option is not used then read item 9 for structured input

9. **IFNOD IGWLAY IGWROW IGWFCOL IFCON FSKIN FLENGW FANISO ICGWADI**
   Item 9 is read for each CLN node to porous medium grid-block connection in the domain. Therefore, item 9 is repeated NCLNGWC times for each of the NCLNGWC connections.

Items 10a or 10b are required for heat transport simulation where BHE detail input is not required (BHEDETAIL is specified as one of the options under OPTION2).

10a. ICONDUITYP FRAD CONDUITK

Item 10a is read for each circular conduit categorized in the model. Therefore, item 10a is repeated NCONDUITYP times for each of the NCONDUITYP types of circular conduit geometries in the model.

10b. IRECTYP FLENGTH FHEIGHT CONDUITK

Item 10b is read for each rectangular conduit categorized in the model. Therefore, item 10b is repeated NRECTYP times for each of the NRECTYP types of rectangular geometries in the model.

Items 10c or 10d are required for heat transport simulation with BHE detail input required (BHEDETAIL is specified as one of the options under OPTION2).

10c. ICONDUITYP FRAD CONDUITK TCOND TTHK TCFLUID TCONV

Item 10c is read for each circular conduit categorized in the model. Therefore, item 10c is repeated NCONDUITYP times for each of the NCONDUITYP types of circular conduit geometries in the model.

10c. IRECTYP FLENGTH FHEIGHT CONDUITK TCOND TTHK TCFLUID TCONV

Item 10d is read for each rectangular conduit categorized in the model. Therefore, item 10d is repeated NRECTYP times for each of the NRECTYP types of rectangular geometries in the model.

11. IBOUND(NCLNNDS) – U1DINT

12. STRT(NCLNNDS) – U1DREL

If ITRNSP is not zero then read items 13 through 16 for transport simulations.

Items 13 through 16 are required for transport simulation and should not be entered for only a flow simulation.

Read Item 13 only if ICBNDFLG = 0

13. [ICBUND(NCLNNDS)] – U1DREL

Read items 14 and 15 only if IDISP is not zero.

14. [DLL(NCLNNDS)] – U1DREL

15. [DLM(NCLNNDS)] – U1DREL

Items C and 16 through 18 below are read for the first component, followed by the next till all NTCOMP contaminant species are read.

Read item C only if the SPATIALREACT option is turned on in the BCT input file. This option allows for spatially distributed reaction stoichiometry between species which may happen if the decay mechanisms are different in different parts of a domain.

C. [SPTLRCT(NCLNNDS,ICOMP,MCOMP)] – U1DREL. Read one array for each layer till all layers are read, then for all parent components of this component ICOMP including the component itself (with a value of zero).

16. [ZODRW (NCLNNDS)] – U1DREL

17. [FODRW (NCLNNDS)] – U1DREL

18. [CONC(NCLNNDS)] – U1DREL

Explanation of Variables Read by the CLN Package

OPTIONS are keyword options. "OPTIONS" must be listed as the first keyword in order to specify any options. The following options are supported:

TRANSIENT indicates that transient IBOUND information will be read for each stress period.

PRINTIAJA will print the IA_CLN and JA_CLN arrays to the listing file. These arrays correspond with the CLNCLN flows that are written to the CLN cell-by-cell output file.

NCLN—is a flag or the number of CLN segments (a segment is defined here as a collection of linearly connected CLN nodes) simulated in the model.

If **NCLN = 0**, this flag indicates that the CLN domain connectivity is input in a general IA-JA manner as is used for the GWF Process.

If **NCLN > 0**, linear CLN segments (for instance multi-aquifer wells) or simple CLN networks are simulated and NCLN is the total number of CLN segments in the domain.

ICLNNDS—is a flag or number of CLN-nodes simulated in the model. Multiple CLN-nodes constitute a segment.

If **ICLNNDS < 0**, the CLN-nodes are ordered in a sequential manner from the first CLN node to the last CLN node. Therefore, only linear CLN segments are simulated since a CLN segment does not share any of its nodes with another CLN segment.

If **ICLNNDS > 0**, CLN networks can be simulated and ICLNNDS is the total number of CLN-nodes simulated by the model. CLN nodes can be shared among CLN segments in the network and therefore, the CLN-nodal connectivity for the network is also required as input.

Note that if NCLN is zero, then ICLNNDS is the total number of CLN nodes in the model (even if the sign is negative).

ICLNCB—is a flag and a unit number.

If **ICLNCB > 0**, cell-by-cell flow terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control. The terms that are saved are storage, and flow between adjacent cells.

If **ICLNCB = 0**, cell-by-cell flow terms will not be written.

If **ICLNCB < 0**, cell-by-cell flow for CLN cells will be written in the listing file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control.

ICLNHD—is a flag and a unit number.

If **ICLNHD > 0**, head output for CLN-nodes will be written to this unit number.

If **ICLNHD = 0**, head output for CLN-nodes will not be written.

If **ICLNHD < 0**, head output for CLN-nodes will be written to the same unit number (IHEDUN) as used for head output for the porous matrix nodes.

ICLNDD—is a flag and a unit number.

If **ICLNDD > 0**, drawdown output for CLN-nodes will be written to this unit number.

If **ICLNDD = 0**, drawdown output for CLN-nodes will not be written.

If **ICLNDD < 0**, drawdown output for CLN-nodes will be written to the same unit number (IDDNUN) as used for drawdown output for the porous matrix nodes.

ICLNIB—is a flag and a unit number.

If **ICLNIB > 0**, IBOUND output for CLN-nodes will be written to this unit number.

If **ICLNIB = 0**, IBOUND output for CLN-nodes will not be written.

If **ICLNIB < 0**, IBOUND output for CLN-nodes will be written to the same unit number (IBOUUN) as used for IBOUND output for the porous matrix nodes.

NCLNGWC—is the number of CLN to porous-medium grid-block connections present in the model. A CLN node need not be connected to any groundwater node. Conversely, a CLN node may be connected to multiple groundwater nodes, or multiple CLN nodes may be connected to the same porous medium mode.

NCONDUITYP—is the number of circular conduit-geometry types that are present within the model.

[OPTIONS2] — include keywords and additional data that are required for different cross-sectional geometries (rectangular cross-sections are currently included), and for turbulent flow simulations using the Darcy-Weisbach equation within the CLN domain. These data are not required if Darcy-Weisbach equation is not used for any of the CLN domain cells and may then be omitted. Additional information may also be required for formatting the cell-by-cell flow files.

RECTANGULAR nrectyp —is a flag indicating that rectangular cross-sectional geometries are included, and the value of “nrectyp” is the number of rectangular-geometry types that are present within the model.

BHEDETAIL —is a flag indicating that BHE details are also included in a heat transport model. Specifically, the thermal conductance and BHE tube thickness are included in

transfer of heat between groundwater and CLN cells along with the heat conductivity of the BHE fluid and the convective heat transfer coefficient.

SAVECLNCON iclncn —is a flag indicating that CLN concentration output is to be saved and the value of "iclncn" is a flag and a unit number.

If **ICLNCN > 0**, concentration output for CLN-nodes will be written to this unit number.
If **ICLNCN = 0**, concentration output for CLN-nodes will not be written.
If **ICLNCN < 0**, concentration output for CLN-nodes will be written to the same unit number (ISPCUN) as used for concentration output for the porous matrix nodes.
Note that if this option does not exist then CLN concentrations are not saved.

SAVECLNMAS iclnmb —is a flag indicating that CLN mass flux output is to be saved and the value of "iclnmb" is a flag and a unit number.

If **ICLNMB > 0**, mass flux output for CLN-nodes will be written to this unit number.
If **ICLNCN = 0**, mass flux output for CLN-nodes will not be written.
If **ICLNCN < 0**, mass flux output for CLN-nodes will be written to the same unit number (IBCTCB) as used for mass flux output for the porous matrix nodes.
Note that if this option does not exist then CLN mass fluxes are not saved.

GRAVITY grav—is the gravitational acceleration constant in model simulation units [L/T^2]. The value of the constant follows the keyword GRAVITY. Note that the constant value is 9.81 m/s^2 in SI units; 32.2 ft/s^2 in fps units. Users should convert the units to a consistent set of units as used in their model.

VISCOSITY visk—is the kinematic viscosity of water in model simulation units [L2/T]. The value of kinematic viscosity follows the keyword VISCOSITY. Note that the constant value is 1.787 x 10^{-6} m^2/s in SI units; 1.924 x 10^{-5} ft^2/s in fps units. Users should convert the units to a consistent set of units as used in their model.

NNDCLN—is the number of CLN-nodes that are associated with each CLN segment.

CLNCON—are the CLN-node numbers associated with each CLN segment.

NJA_CLN—is the total number of connections of the CLN domain. NJA_CLN is used to dimension the sparse matrix in a compressed row storage format.

IAC_CLN—is a matrix indicating the number of connections plus 1 for each CLN node to another CLN node. Note that the IAC_CLN array is only supplied for the CLN cells; the IAC_CLN array is internally expanded to include other domains if present in a simulation.

JA_CLN—is a list of CLN cell number (n) followed by its connecting CLN cell numbers (m) for each of the m CLN cells connected to CLN cell n. This list is sequentially provided for the first to the last CLN cell. Note that the cell and its connections are only supplied for the CLN cells and their connections to the other CLN cells using the local CLN cell numbers. Also note that the JA_CLN list input may be chopped up to have every node number and its connectivity list on a separate line for ease in readability of the file. To further ease readability of the file, the node number of the cell whose connectivity is subsequently listed, may be expressed as a negative number the sign of which is subsequently corrected by the code.

IFNO—is the node number for the CLN node. CLN-nodes are numbered from 1 to the total number of CLN-nodes, NCLNNDS.

IFTYP—is the type-index for the CLN node. The type-index identifies this CLN segment type from the catalogue of CLN elements in a simulation. CLN types include different cross-section shapes (currently only circular conduit geometries are included) of different sizes.

IFDIR—is a directional index for the CLN-node orientation.

If **IFDIR = 0**, the CLN-node is oriented in the vertical direction.

If **IFDIR = 1**, the CLN-node is oriented in the horizontal direction.

If **IFDIR = 2**, the CLN-node is oriented at an angle to the horizontal and the angle is read in parameter FANGLE.

Note that the parameter IFDIR is utilized only to determine a CLN-node's fractional saturation to determine transients or dry conditions.

FLENG—is the length of the CLN-node segment

FELEV—is the elevation of the bottom of the CLN-node.

FANGLE—is the angle made by a CLN-node segment from the horizontal. FANGLE is ignored if the parameter IFDIR is not equal to 2.

IFLIN—is a flag indicating flow conditions within the CLN network. A positive value of IFLIN indicates that the CLN node is treated as confined. If this is an upstream location, the relative permeability is fixed at unity and does not diminish to zero as the CLN cells dewaters and becomes dry. This is similar to the "confined flow" option in the GW domain of MODFLOW. If IFLIN is negative, then flow through the CLN cell is treated as unconfined using the upstream weighted scheme.

If **IFLIN = 0**, flow in the CLN network at this cell is treated as laminar, unconfined (same as if IFLIN = -1).

If the magnitude of IFLIN = 1, the CLN-node is treated as laminar flow.

If the magnitude of IFLIN = 2, the CLN-node is treated as turbulent flow using the Darcy-Weisbach equation.

If the magnitude of IFLIN = 3, the CLN-node is treated as turbulent flow using the Hazen-Williams equation.

If the magnitude of IFLIN = 4, the CLN-node is treated as turbulent flow using the Manning's equation.

ICCWADI—is a flag indicating if vertical flow correction is applied to CLN-CLN flow at this node if it is dry.

If **ICCWADI = 0**, flow in the CLN network at this cell is treated without vertical flow correction.

If **ICCWADI = 1**, vertical flow correction is applied for flow within the CLN network to this node if it is dry.

X1 Y1 Z1 X2 Y2 Z2—are the x, y, and z coordinates of the two ends of a CLN segment. These coordinate inputs are optional and not used by the code. However, they are useful to provide a location to draw the CLN cells within GUIs. GUIs may use only 2-D x and y coordinates as needed.

IFNOD—is the node number for the CLN node that is connected to the groundwater node.

IGWNOD—is the node number of the connecting subsurface node for unstructured grid input.

IGWLAY—is the layer number of the connecting subsurface node, for structured input.

IGWROW—is the row number of the connecting subsurface node, for structured input.

IGWCOL—is the column number of the connecting subsurface node, for structured input.

IFCON—is an index for determining the connectivity equation between CLN-node and its associated matrix node.

If **IFCON = 0**, the Thiem equation is used to provide the connection between CLN-node and matrix node as was done in the Multi-Node Well Package of MODFLOW-2005, without any skin effects.

If **IFCON = 1**, the Thiem equation is used to provide the connection between CLN-node and matrix node as was done in the Multi-Node Well Package of MODFLOW-2005, with inclusion of skin effects.

If IFCON = 2, the connection between CLN-node and matrix node is computed across a leakance term as done in the Conduit Flow Process Package of MODFLOW-2005, with leakance input to the model.

If **IFCON = 3**, the connection between CLN-node and matrix node is computed across a leakance term as done in the Conduit Flow Process Package of MODFLOW-2005, with skin conductivity and skin thickness input to the model and leakance computed internally as per CLN cross-sectional geometry.

If IFCON = 4, the Thiem equation is used to provide the connection between CLN-node and matrix node as was done in the Multi-Node Well package with inclusion of skin effects, however, the skin factor is approximated internally by the code via input of well efficiency (input as FSKIN parameter next).

FSKIN—This parameter determines the leakance across a skin, depending on which equation is selected to represent the flow between CLN cell and matrix.

If **IFCON=0**, the value of FSKIN is ignored and the skin resistance is taken as zero.

If **IFCON=1**, the value of FSKIN is the skin factor for a CLN-matrix connection that uses the Thiem Equation with skin resistance.

If **IFCON=2**, the value of FSKIN is the leakance of the sediments (skin) between the CLN and the matrix node for a CLN-matrix connection as used in the Conduit Flow Process Package of MODFLOW-2005.

If **IFCON=3**, the value of FSKIN is the hydraulic conductivity of the sediments (skin) between the CLN node and the matrix for computing the CLN-matrix leakance as used in the Conduit Flow Process Package of MODFLOW-2005.

If IFCON=4, the value of FSKIN is the well efficiency for a CLN-matrix connection that uses the Thiem Equation with skin resistance. Note that efficiency is entered as a fraction ranging from 0 to 1.

FLENGW—is the length of the connection between the CLN cell and the GW cell.

FANISO—This parameter is used in computation of leakance across a skin, depending on which equation is selected to represent the flow between CLN node and matrix.

If **IFCON=0 or 1**, the value of FANISO is the anisotropy factor of the porous matrix block that is connected to the CLN-node, used for computations related to the Thiem Equation. The Kx/Ky value is provided here for a vertically oriented CLN cell, and Kx/Kz is provided here for a horizontally oriented CLN cell. These anisotropies may or may not be read in the BCF or LPF packages depending on the selected simulation options, and are therefore input here to accommodate anisotropic computations for flow to wells. This input therefore provides independent control of flow to wells in anisotropic media.

If **IFCON=2**, the value of FANISO is not used.

If **IFCON=3**, the value of FANISO is the thickness of sediments (skin) between the CLN and matrix nodes for computing the CLN-matrix leakance as used in the Conduit Flow Process Package of MODFLOW-2005.

ICGWADI—is a flag indicating if vertical flow correction is applied to CLN-GW flow at this node if either cell is dry.

If **ICGWADI = 0**, CLN-GW flow at this cell is treated without vertical flow correction.

If **ICGWADI = 1**, vertical flow correction is applied for CLN-GW flow at this node if it is dry.

FLENGW—is the length of the CLN-node's connection with the groundwater node.

ICONDUITYP—is the index for the conduit type.

Note that the next three variables TCOND, TTHK, and TCFLUID are only required for heat transport simulations of BHE operations where the CLNs are used to simulate the BHEs.

TCOND—is the thermal conductivity of the BHE tube. **A high value for TCOND may be provided if resistance to heat flow resulting from the BHE pipe material is not to be considered in the simulation**.

TTHK—is the thickness of the BHE tube.

TCFLUID—is the thermal conductivity of the fluid in the BHE tube which may be different from the thermal conductivity of water in the porous medium for a closed system. An effective value may be entered to account for a different heat capacity and density than that of water. The effective value results by multiplying the fluid heat conductivity by its density and heat capacity and dividing by the density and heat capacity of water. ***A negative input value for fluid heat capacity indicates that the BHE fluid is water and the thermal properties for water entered in the BCT package will be used***.

TCONV—is the thermal convective coefficient of the BHE tube. **A value of zero may be entered if this effect is not to be simulated by the code**.

FRAD—is the radius of the circular conduit type.

IRECYP—is the index for the rectangular geometry type.

FWIDTH—is the width of the rectangular geometry type.

FHEIGHT—is the height of the rectangular geometry type.

CONDUITK—is the hydraulic conductivity or resistance factor of the conduit. The value that is entered depends on the equation being used to solve for flow through the conduit.

If the magnitude of IFLIN = 1, or if IFLIN = 0, the CLN flow is treated as laminar, and CONDUITK represents the laminar conductance term of the CLN segment expressed as $ConduitK = (\rho g / 8\mu)$. Note that CONDUITK times radius squared is used to compute the effective hydraulic conductivity of the conduit, as per laminar flow equation. CONDUITK has dimensions of [1/LT].

If the magnitude of IFLIN = 2, the CLN-node is treated as turbulent flow using the Darcy-Weisbach equation, and CONDUITK represents the mean roughness height of the CLN surface [L].

If the magnitude of IFLIN = 3, the CLN-node is treated as turbulent flow using the Hazen-Williams equation, and CONDUITK represents the Hazen-Williams factor for relative roughness of the CLN surface [$L^{0.37}/T$].

If the magnitude of IFLIN = 4, the CLN-node is treated as turbulent flow using the Manning's equation, and CONDUITK represents the Manning's coefficient for relative roughness of the CLN surface [$T/L^{(1/3)}$].

NCLNNDS—is the total number of CLN-nodes. This parameter is computed internally by the code.

$$NCLNNDS = ICLNNDS \qquad for \qquad ICLNNDS \geq 0$$

$$NCLNNDS = \sum_{NLFF} NNDCLN(NCLN) \qquad for \qquad ICLNNDS < 0$$

IBOUND—is the boundary array for CLN-nodes.

If **IBOUND(IFN) < 0**, CLN-cell IFN has a constant head.

If **IBOUND(IFN) = 0**, CLN-cell IFN is no flow.

If **IBOUND(IFN) > 0**, CLN-cell IFN is variable head.

STRT—is initial (starting) head—that is, head at the beginning of the simulation. STRT must be specified for all simulations, including steady-state simulations. One value is read for every CLN cell.

ICBUND—is the active or inactive flag for transport for the CLN-nodes.

DLL—is the dispersion coefficient along the conduit-node direction, if transport is simulated.

DLM—is the dispersion coefficient for the conduit-node flow to/from the porous matrix, if transport is simulated.

SPTLRCT—is a real array of location dependent stoichiometric coefficients indicating mass units of ICOMP generated due to decay of one mass unit of parent JPARENT. This is provided for every node if the SPATIALREACT option is invoked. First, the value of SPTLRCT is read for all CLN cells of the first parent component, then for the next, till all NPARENT component stoichiometric coefficients are defined at all CLN cells within the domain.

ZORDW—is the zeroth order decay coefficient for a species in the CLN cell.

FORDW—is the first order decay coefficient for a species in the CLN cell.

CONC—is the initial concentration of species at the conduit-node.

BLOCK CENTERED TRANSPORT PACKAGE INPUT INSTRUCTIONS

A BCT package input file is read for every transport simulation. The BCT package input includes all storage, decay, and transport related parameters necessary to conduct a species transport simulation. A boundary condition file is also included for prescribed concentration boundaries. For flow related boundaries, a third type boundary condition is applied by supplying the concentration of inflowing water as auxiliary variables in the respective boundary package input files. For outflow nodes, this concentration is not required and is ignored if input. Further details on input of auxiliary variables for concentrations within the respective boundary files are provided in the sub-section titled “Model Input and Output” under the “Implementation and Program Design” section. Additional input required for transport simulations are discussed below.

Input for the Block Centered Transport (BCT) Package is read from the file that is type "BCT" in the Name File. The BCT Package input instructions include flags, indices, transport related parameters and initial conditions for solution to transport of contaminants in a steady-state or transient flow field. The input is read in a free format.

The BCT package has been updated since its first release, with additional options and heat simulation capability. It should be noted that additions have been made in a backward compatible manner and therefore earlier versions of the input instructions without those capabilities would also work.

The BCT Package performs transport for solutes as well as for heat. The flag IHEAT turns on a **heat transport** simulation. If solute transport is also active, then heat is the component after all MCOMP mobile solute components.

Adsorption of solutes on the air-water interface is also included using the A-W_ADSORB option. This feature is meant to accommodate PFAS and related compounds that are surfactant-like and may be held back on the air-water interface in the vadose zone. The option is meant to be used with simulating Richards' equation for saturated / unsaturated flow. PFAS compounds may also have an impact on the air-water capillarity thus affecting the moisture retention curves. Furthermore, PFAS solutions can have a wide range of viscosities that may affect flow. These impacts may be included by adjusting the van Genuchten parameters and the viscosity in a time-lagged manner but are neglected in the code for now.

The BCT package is also set up to compute reactions among solute components in an iteratively coupled manner. For such reactions, there could be immobile components which partake in reactions but not in solute transport. Immobile solute components may be added via the counter IMCOMP. The immobile components are ordered after all mobile components (and the heat equation if also solved). Also, the sequential iterations between transport and reactions may be controlled by a sequential iteration counter NSEQITR. Note this discussion is about mobile and immobile solute components (and not about mobile and immobile domains of a dual domain conceptualization).

A **solubility limit** to concentrations is also included via the option SOLUBILITY. Formulation details are provided earlier in the "Solubility" subsection. If the SOLUBILITY option is used, then

a solubility limit and a linear equilibrium partitioning coefficient for solutes in a precipitated phase are also included as input.

An option (**ONLY_SATADSORB**) is provided for unconfined situations where adsorption of solute is not over the entire grid-block but only over the saturated thickness (up to the water table) of the grid block. The saturated thickness of the first time-step of the first stress period is used if the flow is transient. This approximation does not allow adsorption sites to change with the saturated thickness but it allows for a mass conserved solution for transient flow situations where the cell size and the saturated cell size can differ greatly.

A **time-weighting** option has also been included to allow greater accuracy with temporal discretization. The TIMEWEIGHT option includes a weighting factor to be entered. A weighting factor of 1 is fully implicit weighting which is the default. A weighting factor of 0.5 weights some of the terms in a Crank-Nicolson manner which increases the temporal accuracy of solution and is also unconditionally stable for fully upstream weighting. Crank-Nicolson weighting may not however maintain the TVD property. Therefore, smaller time-step sizes or higher temporal weighting should be used in case oscillations occur with temporal weighting. Using a weighting factor less than 0.5 is not recommended.

Several additional flags and options have also included for transport simulations to provide flexibility with simulations and with output. **The ITRNSP = 2 flag has been activated to allow transport simulations to be performed after successful completion of the flow simulation.** This option skips the solution for heads altogether, and instead reads the output binary heads (HDS) file from the pre-run flow simulation, computes all the necessary saturations, fluxes and mass balances, and proceeds directly to a transport simulation for each time step. Note that precision may be lost with this option due to reading of the binary HDS file.

Often, a transport simulation in a steady-state flow field may require transient transport boundary conditions. A simulation would then include multiple stress periods to change the boundary conditions as needed. However, if flow is steady state, the flow equation is solved at every time with associated wasted computations since nothing changes in the flow field. **An option for ITRNSP = 3 has been included that would skip flow computations *after* the first time-step of the first stress period.** This would allow for transient transport boundary conditions to be provided using multiple stress periods efficiently, in a steady-state flow field. An option to set the **flag ITRNSP = 4 allows for the heads to be read from a pre-run flow simulation for only**

the first time-step (like for ITRNSP = 2), with remaining time steps and stress periods allowing transient transport boundary conditions (like for ITRNSP = 3).

Finally, an option to set the **flag ITRNSP = 5 is a special case that helps with initialization of simulations with matrix diffusion**. For that case, the flow simulation is bypassed for eah stress period and transport only is run with the initial concentrations treated as prescribed concentrations at each node. This allows for "bleeding in" of the solutes from the fracture domain to the matrix domain of the MDT process. Different concentrations can be provided for multiple stress periods to allow concentrations to bleed in and out of the MDT domain for estimated plume shapes at different times in the past, to create initial conditions. The MDT domain uses an analytical solution, therefore, there is no specific value of concentration that can be assigned to the matrix domain since the concentrations are not uniform. The bleeding in process creates concentration profiles within the matrix domain for estimated plumes of the past.

An option is provided to **write concentration output to separate binary files** when a simulation is for multiple species. By default, all species output is to the same one binary file on ICONUN in the output control input. The "MULTIFILE" option attaches the words species number for each species to the root file name. This is done for CLN and matrix domain as well if these domains are included in a simulation.

FOR EACH SIMULATION

1a. ITRNSP IBCTCB MCOMP ICBNDFLG ITVD IADSORB ICT CINACT CICLOSE IDISP IXDISP DIFFNC IZOD IFOD IFMBC IHEAT IMCOMP IDISPCLN NSEQITR [OPTIONS]

These twelve variables are free format if the option "FREE" is specified in the Basic Transport Package input file; otherwise, the variables all have 10-character fields.

Read item 1b below, ONLY if IFMBC = 1 indicating that flow mass balance errors will be evaluated and incorporated into the transport solution. The data in item 1b below provides unit numbers for output of the results. Note that the NAME file should also include these unit numbers and open appropriate files for the GW and CLN domains. Suggested extensions for the files are FMG (flow mass balance for groundwater domain), TMG (transport mass balance for groundwater domain), FMC (flow mass balance for CLN domain), and TMC (transport mass balance for CLN domain).

1b. MBEGWUNF MBEGWUNT MBECLNUNF MBECLNUNT

If IFMBC in item 1a above is zero then item 1b is not read.

1c. HTCONDW RHOW HTCAPW

If IHEAT in item 1a above is zero then item 1c is not read.

1d. NAZONES NATABROWS – Format free. The variable **nazones** represents the number of soil zones, and the variable **natabrows** indicates the number of rows of tabular input to define the function for the air-water interface area, or the air-water interface partitioning coefficient, or both.

Read item 1d only if AW_ADSORB option in item 1a above is used and either flag IAREA_FN = 5 or IKAWI_FN = 4 (i.e., tabular input is used for the area or Kaw functions).

1e. [IAWIZONMAP(NODES)] -- U1DINT. Read one integer array for all groundwater nodes.

Read item 1e only if AW_ADSORB option in item 1a above is used and either flag IAREA_FN = 5 or IKAWI_FN = 4 (i.e., tabular input is used for the area or Kaw functions).

1f. ROG_SIGMA

Read item 1f only if AW_ADSORB option in item 1a above is used and the flag IAREA_FN = 3.

1g. SIGMA_RT

Read item 1g only if AW_ADSORB option in item 1a above is used and the flag IKAWI_FN = 3.

1h. [AWI_AREA_TAB(SAT, AREA)] – One row for each of the "**natabrows**" of a table, which is then repeated "**nazones**" times for each soil zone in the catalogue.

Read item 1h only if AW_ADSORB option in item 1a above is used and flag IAREA_FN = 5. (i.e., tabular input is used for the area-saturation function). Item 1h has natabrows times nazones the number of entries where each entry is the area for a given saturation in the saturation – area function.

If UNSTRUCTURED option is used, then read items 2 through 20.

A subset of the following one-dimensional variables is used to describe each node. The variables needed for each node depend on the transport options that are selected. Unneeded variables must be omitted.

The required variables for each of Items 2 – 4 and items 6 – 20 for layer 1 are read first; then for layer 2 and so forth. The next variable of Items 2 – 4 and items 6 – 20 is read after all layers for the previous variable are read. Note that there may be different number of nodes per layer (NDSLAY) for an unstructured grid.

If ICBNDFLG is zero then read item 2.

2. **[ICBUND(NDSLAY)] – U1DINT. Read one array for each layer till all layers are read.**
3. **[PRSITY(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read.**

   If IADSORB is not zero **OR if IHEAT is not zero** then read item 4.

4. **[BULKD(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read.**

   If IDISP is not zero then read item 5.

5. **[ANGLEX(NJA)] – U1DREL.**

   If IDISP is equal to one then read items 6 and 7.

6. **[DL(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read.**
7. **[DT(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read.**

   If IDISP is equal to two then read items 8, 9, 10, 11, 12 and 13.

8. **[DLX(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read.**
9. **[DLY(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read.**
10. **[DLZ(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read.**
11. **[DTXY(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read.**

12. **[DTYZ(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read.**

13. **[DTXZ(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read.**

If IHEAT is equal to ONE then read the following items H1 and H2.

H1. [HTCAPS(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read. Note that the soil heat capacity is actually read in array ADSORB as the adsorption term in solute transport is equivalent to the soil heat storage of the energy equation.

H2. [HTCONDS(NDSLAY)] – U1DREL. Read one array for each layer till all layers are read.

If AW_ADSORB option is on then read the following items A1, through A5, depending on the option selected to compute interfacial area for air-water interface adsorption.

Read item A1 if IAREA_FN is 1.

A1. AWAMAX(NDSLAY) – U1DREL. Read one array for each layer till all layers are read.

Read item A2 if IAREA_FN is 2.

A2. GRAIN_DIA(NDSLAY) – U1DREL. Read one array for each layer till all layers are read.

Nothing is read here when IAREA_FN is 3 as AWAMAX is computed internally using ROG_SIGMA read in 1f above, and the porosity. **Note that IAREA_FN = 3 is currently not available.**

Read item A3, A4 and A5 if IAREA_FN is 4.

A3. AWAREA_X2(NDSLAY) – U1DREL. Read one array for each layer till all layers are read.

A4. AWAREA_X1(NDSLAY) – U1DREL. Read one array for each layer till all layers are read.

A5. AWAREA_X0(NDSLAY) – U1DREL. Read one array for each layer till all layers are read.

Nothing is read here when IAREA_FN is 5 as tabular function input for area v saturation is done earlier in 1h.

Items 14 – 20 (and S1 and S2 and also optionally C1 through C3 below, and optionally items A6 through A8 below) are read for the first component, followed by the next, till all mobile MCOMP transport species are read. If heat equation is also solved, it is the MCOMP+1th input for item 20 where the temperature is read in the concentration array.

If SOLUBILITY option is on then read the following items S1, and S2.

S1. SOLLIM(ICOMP) – U1DREL. Read one array for all mobile components.

S2. SOLSLOPE(ICOMP) – U1DREL. Read one array for all mobile components.

If CHAINDECAY option is on then read the following items C1, C2 and C3.

C1. [NPARENT(ICOMP)] - Integer Number.

Read items C2 and C3 only if NPARENT of this component is greater than zero

C2. [JPARENT(ICOMP,MCOMP)] – U1DINT. Read one array for all mobile components including the component itself (with a value of zero).

Read item C3 only if the SPATIALREACT option is NOT turned on.

C3. [STOTIO(ICOMP,MCOMP)] – U1DREL. Read one array for all mobile components including the component itself (with a value of zero).

Read item C4 only if the SPATIALREACT option is turned on.

C4. [SPTLRCT(NDSLAY,ICOMP,NPAREN)] – U1DREL. Read one array for each layer till all layers are read, then for all parent components of this component ICOMP till all NPAREN = JPARENT(ICOMP,MCOMP) components are read for ICOMP.

If AW_ADSORB option is on, then read the following items A6, A7 and A8.

Read items A6 and A7 only if flag IKAWI_FN = 1, 2, or 3.

A6. [ALANGAW(NDSLAY,ICOMP)] – U1DREL. Read one array for each layer till all layers are read.

A7. [BLANGAW(NDSLAY,ICOMP)] – U1DREL. Read one array for each layer till all layers are read.

Read item A8 only if flag IKAWI FN = 4. (i.e., tabular input is used for the Kaw-Concentration function).

A8. [AWI_KAWI_TAB(CONC, KAWI, ICOMP)] – One row for each of the "**nutabrows**" of a table, which is then repeated "**nuzones**" times for each soil zone in the catalogue.

Item A8 has nutabrows times nuzones the number of entries where each entry is the adsorption coefficient for a given concentration of this solute in the concentration – K_{awi} function.

If IADSORB is not zero then read item 14.

14. [ADSORB(NDSLAY,ICOMP)] – U1DREL. Read one array for each layer till all layers are read.

If IADSORB is two or three then read item 15.

15. [FLICH(NDSLAY,ICOMP)] – U1DREL. Read one array for each layer till all layers are read.

If IZOD is one or three or four, then read item 16.

16. [ZODRW(NDSLAY,ICOMP)] – U1DREL Read one array for each layer till all layers are read.

If IADSORB is not zero and IZOD is two or three or four, then read item 17

17. [ZODRS(NDSLAY,ICOMP)] – U1DREL Read one array for each layer till all layers are read.

If IAW_IADSORB is not zero and IZOD is four, then read item 17a

17a. [ZODRAW(NDSLAY,ICOMP)] – U1DREL Read one array for each layer till all layers are read.

If IFOD is one or three or four, then read item 18

18. [FODRW(NDSLAY,ICOMP)] – U1DREL Read one array for each layer till all layers are read.

If IADSORB is not zero and IFOD is two or three or four, then read item 19

19. [FODRS(NDSLAY,ICOMP)] – U1DREL Read one array for each layer till all layers are read.

If IAW_IADSORB is not zero and IFOD is four, then read item 19a

19a. [FODRAW(NDSLAY,ICOMP)] – U1DREL Read one array for each layer till all layers are read.

20. [CONC(NDSLAY,ICOMP)] – U1DREL. Read one array for each layer till all layers are read. For heat transport, the temperature is also read in this variable itself. The "EXPLANATION OF VARIABLES" section below details the order of solute species and temperature.

Otherwise, if UNSTRUCTURED option is not used then read items 21 through 33 for structured input.

A subset of the following two-dimensional variables is used to describe each layer. The variables needed for each layer depend on the transport options that are selected. Unneeded variables must be omitted.

The required variables for each of Items 21 – 33 for layer 1 are read first; then for layer 2 and so forth. The next variable of Items 21 – 33 is read after all layers for the previous variable are read.

If ICBNDFLG is zero then read item 21

21. [ICBUND(NCOL,NROW)] -- U2DINT. Read one array for each layer till all layers are read.

22. **[PRSITY(NCOL,NROW)] -- U2DREL. Read one array for each layer till all layers are read.**

    If IADSORB is not zero then read item 23

23. **[BULKD(NCOL,NROW)] -- U2DREL Read one array for each layer till all layers are read.**

    If IDISP is equal to one, then read items 24 and 25

24. **[DL(NCOL,NROW)] -- U2DREL Read one array for each layer till all layers are read.**

25. **[DT(NCOL,NROW)] -- U2DREL Read one array for each layer till all layers are read.**

    If IDISP is equal to two, then read items 26, 27 28, 29, 30 and 31.

26. **[DLX(NCOL,NROW)] -- U2DREL Read one array for each layer till all layers are read.**

27. **[DLY(NCOL,NROW)] -- U2DREL Read one array for each layer till all layers are read.**

28. **[DLZ(NCOL,NROW)] -- U2DREL Read one array for each layer till all layers are read.**

29. **[DTXY(NCOL,NROW)] -- U2DREL Read one array for each layer till all layers are read.**

30. **[DTYZ(NCOL,NROW)] -- U2DREL Read one array for each layer till all layers are read.**

31. **[DTXZ(NCOL,NROW)] -- U2DREL Read one array for each layer till all layers are read.**

If IHEAT is equal to ONE then read the following items H3 and H4.

H3. [HTCAPS(NCOL,NROW)] – U1DREL. Read one array for each layer till all layers are read. Note that the soil heat capacity is actually read in array ADSORB as the adsorption term in solute transport is equivalent to the soil heat storage of the energy equation.

H4. [HTCONDS(NCOL,NROW)] – U1DREL. Read one array for each layer till all layers are read.

If AW_ADSORB option is on then read the following items A9, through A13, depending on the option selected to compute interfacial area for air-water interface adsorption.

Read item A9 if IAREA_FN is 1.

A9. AWAMAX(NCOL,NROW) – U1DREL. Read one array for each layer till all layers are read.

Read item A10 if IAREA_FN is 2.

A10. GRAIN_DIA(NCOL,NROW) – U1DREL. Read one array for each layer till all layers are read.

Nothing is read here when IAREA_FN is 3 as AWAMAX is computed internally using ROG_SIGMA read in 1f above, and the porosity.

Read item A11, A12 and A13 if IAREA_FN is 4.

A11. AWAREA_X2(NCOL,NROW) – U1DREL. Read one array for each layer till all layers are read.

A12. AWAREA_X1(NCOL,NROW) – U1DREL. Read one array for each layer till all layers are read.

A13. AWAREA_X0(NCOL,NROW) – U1DREL. Read one array for each layer till all layers are read.

Nothing is read here when IAREA_FN is 5 as tabular function input for area v saturation is done earlier in 1h.

If SOLUBILITY option is on then read the following items S3, and S4.

S3. SOLLIM(ICOMP) – U1DREL. Read one array for all mobile components.

S4. SOLSLOPE(ICOMP) – U1DREL. Read one array for all mobile components.

Items 32 – 38 (and optionally C1 through C3 below) are read for the first component, followed by the next, till all MCOMP mobile transport species are read. If heat equation is also solved, it is the MCOMP+1th input for item 38 where the temperature is read in the concentration array.

If CHAINDECAY option is on then read the following items C5, C6 and C7. Also read item C8 if in addition, the

C5. [NPARENT(ICOMP)] - Integer Number.

C6. [JPARENT(ICOMP,MCOMP)] – U1DINT. Read one array for all mobile components including the component itself (with a value of zero).

Read item C7 only if the SPATIALREACT option is NOT turned on.

C7. [STOTIO(ICOMP,MCOMP)] – U1DREL. Read one array for all mobile parent components of this component ICOMP including the component itself (with a value of zero).

Read item C8 only if the SPATIALREACT option is turned on.

C8. [SPTLRCT(NCOL,NROW,ICOMP,MCOMP)] – U1DREL. Read one array for each layer till all layers are read, then for all parent components of this component ICOMP including the component itself (with a value of zero).

If AW_ADSORB option is on, then read the following items A14, A15 and A16.

Read items A14 and A15 only if flag IKAWI_FN = 1, 2, or 3.

A14. [ALANGAW(NCOL,NROW,ICOMP)] – U1DREL. Read one array for each layer till all layers are read.

A15. [BLANGAW(NCOL,NROW,ICOMP)] – U1DREL. Read one array for each layer till all layers are read.

Read item A8 only if flag IKAWI_FN = 4. (i.e., tabular input is used for the Kaw-Concentration function).

A16. [AWI_KAWI_TAB(CONC, KAWI, ICOMP)] – One row for each of the "**nutabrows**" of a table, which is then repeated "**nuzones**" times for each soil zone in the catalogue.

Read item A16 only if AW_ADSORB option in item 1a above is used and flag IKAWI_FN = 4. (i.e., tabular input is used for the Kaw-Concentration function). Item A16 has nutabrows

times nuzones the number of entries where each entry is the adsorption coefficient for a given concentration of this solute in the concentration – K_{awi} function.

If IADSORB is not zero then read item 32

32. **[ADSORB(NCOL,NROW,ICOMP)] -- U2DREL Read one array for each layer till all layers are read.**

    If IADSORB is two or three then read item 33

33. **[FLICH(NCOL,NROW,ICOMP)] -- U2DREL Read one array for each layer till all layers are read.**

    If IZOD is one or three or four, then read item 34

34. **[ZODRW(NCOL,NROW,ICOMP)] -- U2DREL Read one array for each layer till all layers are read.**

    If IADSORB is not zero and IZOD is two or three or four, then read item 35

35. **[ZODRS(NCOL,NROW,ICOMP)] -- U2DREL Read one array for each layer till all layers are read.**

    If IAW_IADSORB is not zero and IZOD is four, then read item 37a

37a. **[ZODRAW(NCOL,NROW,ICOMP)] -- U2DREL Read one array for each layer till all layers are read.**

    If IFOD is one or three or four, then read item 36

36. **[FODRW(NCOL,NROW,ICOMP)] -- U2DREL Read one array for each layer till all layers are read.**

    If IADSORB is not zero and IFOD is two or three or four, then read item 37

37. **[FODRS(NCOL,NROW,ICOMP)] -- U2DREL Read one array for each layer till all layers are read.**

    If IAW_IADSORB is not zero and IFOD is four, then read item 37a

37a. [FODRAW(NCOL,NROW,ICOMP)] -- U2DREL Read one array for each layer till all layers are read.

38. [CONC(NCOL,NROW,ICOMP)] -- U2DREL Read one array for each layer till all layers are read. For heat transport, the temperature is also read in this variable itself. The EXPLANATION OF VARIABLES below details the order of solute species and temperature.

EXPLANATION OF VARIABLES READ BY THE BCT PACKAGE

ITRNSP—is a transport simulation flag

If ITRNSP = 0, then transport is not simulated.

If ITRNSP = 1, then transport is simulated immediately after every flow time step or a steady-state flow simulation.

If ITRNSP = 2, then transport is simulated using the flow field of a previously simulated flow run.

If ITRNSP = 3, then flow computations are skipped after the first time-step of the first stress period. Transport is then simulated using the flow field of the first stress period. This option is useful for supplying transient transport boundary conditions using multiple stress periods, where the flow field is steady state, which is solved in the first time-step of the first stress period.

If ITRNSP = 4, then Transport is then simulated using the flow field of the previous flow run. Furthermore, only the first stress period of flow is read, the remaining stress periods are for supplying transient transport boundary conditions as in ITRNSP = 3. This option is useful for supplying transient transport boundary conditions using multiple stress periods, where the flow field is steady state, which is read from an existing CBC file in the first time-step of the first stress period.

If ITRNSP = 5, then flow computations are skipped entirely, all initial concentrations (of only the mobile domain for dual porosity or matrix diffusion simulations) are set to prescribed concentrations, and transport simulations are performed for a saturated domain with zero

flow. This condition is useful to load up the matrix domain over a given time period of solute existing static in the fracture domain.

If ITRNSP = -1, then this simulation is for capture probability. All the velocities are reversed and simulation is carried out. ITRNSP is reset to 1, and flag ICPROB is set to 1 to indicate further that this is a capture probability simulation, as per Frind and Molson, (2018). E.O. Frind, and J.W. Molson, 2018, Issues and Options in the Delineation of Well Capture Zones under Uncertainty, Groundwater, doi: 10.1111/gwat.12644. ***Note that this option is not currently available.***

IBCTCB—is a flag and a unit number.

If IBCTCB > 0, cell-by-cell mass flux terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control. The terms that are saved are mass storage, mass flux from constant-concentration nodes, and mass flux in or out of the respective boundaries (WEL, DRN, GHB, RIV, STR, CHD, etc.). Note that prescribed concentration boundary (PCB) fluxes can be written to a separate file indexed in the PCB package input. Also note that if the "COMPACT BUDGET" option was selected in the OC package then the compact budget formats will be used.

If IBCTCB = 0, cell-by-cell mass flux terms will not be written.

If IBCTCB < 0, cell-by-cell mass flux for constant-concentration cells will be written in the listing file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control. Cell-by-cell mass flux to storage and between adjacent cells will not be written to any file.

MCOMP—is the number of mobile component species simulated.

ICBNDFLG—is a flag that determines if the active domain for transport is the same as that for flow.

If ICBNDFLG = 0, the active domain for transport is not the same as for flow and is read.

If ICBNDFLG = 1, the active domain for transport is the same as IBOUND for flow and the transport IBOUND array does not need to be read but is set from that of flow.

ITVD—is a flag and counter.

If ITVD = 0, the upstream weighted scheme is used for simulating the advective term.

If ITVD >0, the TVD scheme is used for simulating the advective term, and the value of ITVD represents the number of TVD correction iterations applied to the solution.

IADSORB—is an adsorption flag.

If IADSORB = 0, then adsorption is not simulated.

If IADSORB = 1, then linear adsorption is simulated.

If IADSORB = 2, then Freundlich adsorption is simulated.

If IADSORB = 3, then Langmuir adsorption is simulated.

ICT—is a flag that determines the transport solution scheme.

If ICT = 0, then the transport solution is for water phase concentration.

If ICT = 1, then the transport solution is for total concentration.

Note that when adsorption is very large, a solution to the total concentration (ICT = 1) may be more accurate in capturing the total system mass.

CINACT—is the concentration value that will be output at inactive nodes in the simulation.

CICLOSE—is the concentration tolerance for convergence of the matrix solver.

IDISP—is a flag indicating the dispersion formula used in the model

If IDISP = 0, then dispersion is not simulated.

If IDISP = 1, then isotropic dispersion is simulated.

If IDISP = 2, then anisotropic dispersion is simulated

IXDISP—is a flag indicating if cross-dispersion is simulated

If IXDISP = 0, then cross-dispersion is not simulated.

If IXDISP = 1, then cross-dispersion is included in the model.

DIFFNC—is the molecular diffusion coefficient for contaminant in water. Note that only one diffusion coefficient is read even if there are multiple contaminants simulated. Typically, diffusion is neglected as it is a small component of the overall fate and transport.

IZOD—is a flag indicating if zero order decay is simulated.

If IZOD = 0, then zero order decay is not simulated.

If IZOD = 1, then zero order decay is included in water.

If IZOD = 2, then zero order decay is included on soil if there is adsorption.

If IZOD = 3, then zero order decay is included in water and on soil if there is adsorption.

If IZOD = 4, then zero order decay is included on the air-water interface if there is adsorption onto the air-water interface, along with zero order decay in water and on soil. Note that if zero order decay does not occur in any of the phases, the related coefficient can be set to zero. If there is an air-water interface, with no zero order decay on the air-water interface, the other IZOD options may be used.

IFOD—is a flag indicating if first order decay is simulated

If IFOD = 0, then first order decay is not simulated.

If IFOD = 1, then first order decay is included in water.

If IFOD = 2, then first order decay is included on soil if there is adsorption.

If IFOD = 3, then first order decay is included in water and on soil if there is adsorption.

If IFOD = 4, then first order decay is included on the air-water interface if there is adsorption onto the air-water interface, along with first order decay in water and on soil. Note that if first order decay does not occur in any of the phases, the related coefficient can be set to zero. If there is an air-water interface, with no first order decay on the air-water interface, the other IZOD options may be used.

IFMBC—is a flag indicating if Flux mass balance errors are to be considered in the flow solution and reported for fluid and mass fluxes.

If IFMBC= 0, then flow mass balance errors are not computed and transport does not consider these errors in the solution.

If IFMBC = 1, then flow mass balance errors are computed and transport considers these errors in the solution. Also, these errors are reported for fluid flux and for mass flux in an output file.

IHEAT—is a flag indicating if the energy balance equation is to be solved.

If IHEAT= 0, then energy balance equation is not solved.

If IHEAT = 1, then the energy balance equation is solved. If solute transport is also solved for the simulation, then the heat equation is solved after all mobile solute components are solved.

IMCOMP—is the number of immobile component species in a simulation. These are the species that are tracked, but are not part of the transport equation. These other immobile species may be significant for reaction and geochemical calculations. The order in which species are stored is as follows: First, the mobile MCOMP equations are stored. If heat is also solved, then this is followed by temperature giving a total of MCOMPT transport species (MCOMPT = MCOMP if heat is not solved). Finally, the immobile components (IMCOMP) are stored. Thus, the total number of transport components NTCOMP is equal to MCOMPT plus IMCOMP.

IDISPCLN—is an index for the connection between GWF cell and CLN cell. If there are no CLN cells in the simulation then this index is still read, but ignored.

If IDISPCLN= 0, then all the CLN-GW connection uses the finite difference approximation for dispersion and heat conduction.

If IDISPCLN = 1, then the CLN-GW connection uses the Thiem solution for dispersion and heat conduction.

If IDISPCLN = 2, then the CLN-GW connection uses the Thiem solution for dispersion and heat conduction with a local borehole thermal resistance term. An additional array is then read to provide the borehole thermal resistance which is the net effect of various local (skin, grout, U-tube material) conditions.

NSEQITR—is an index or count for performing sequential iterative iterations over all of the solute transport components. Sequential iterations may be performed if reaction or geochemical modules are attached that impact all of the simulated components.

If NSEQITR = 0 or 1, then no iterations are performed over all component iterations.

If NSEQITR = n (n > 1), then "n" is the number of iterations that will be performed on the transport and reaction modules.

[OPTIONS] — include keywords for various options that may be invoked.

TIMEWEIGHT tw — "TIMEWEIGHT" is a flag indicating that a time weighting of value "tw" should be used for the transport simulation instead of fully implicit default weighting (where tw=1). Note that a time weighting factor between 0.5 and 1.0 may be applied for unconditionally stable solution to the transport equation. A time weighting of 0.5 is the Crank-Nicolson scheme which has a second order accuracy in time as compared to the fully implicit scheme which is first order accurate in time. However, Crank-Nicolson scheme may not be TVD. Therefore, smaller time-step sizes or higher temporal weighting should be used in case oscillations occur with temporal weighting. Using a weighting factor less than 0.5 is not recommended. Note that time weighting is only applied to the advective and dispersive concentration terms while other terms are still maintained fully implicitly.

CHAINDECAY— Indicates that transformation of parent to daughter product is simulated. Additional input will be required to identify parent species and stoichiometric coefficients of the reactions.

ONLY_SATADSORB—This is a keyword that allows for soil adsorption to occur only over the saturated thickness portion of an unconfined aquifer cell instead of the entire cell thickness. The saturated thickness of the first time-step of the first stress period is used if the flow is transient. This approximation does not allow adsorption sites to change with the

saturated thickness but it allows for a mass conserved solution for transient flow situations where the cell size and the saturated cell size can differ greatly.

SPATIALREACT — turns on location variable stoichiometric reactions for a simulation if chain decay is on.

SOLUBILITY — turns on a solubility limit to the concentration of each species. With this option set, the solubility limit and an equilibrium partitioning coefficient are read for each species. If concentration of a solute increases past its solubility limit due to evapotranspiration, species generation, or other mechanisms, the solute will start to precipitate out of solution. The partitioning coefficient allows for an equilibrium mechanism to also control this precipitation to include supersaturation mechanisms to be simulated. Partitioning could also be to/from any non-aqueous phase. The section on "solubility" provides details.

A-W_ADSORB iarea_fn ikawi_fn— The keyword **A-W_ADSORB** indicates that air-water interface adsorption will be simulated with transport. The flags **iarea_fn** and **ikawi_fn** indicate input options for the area v. saturation function, and for the air-water interface partition coefficient Kawi v. concentration function respectively. Options for the area as a function of interfacial saturation include:

Iarea_fn = 1 is when A_{max} is input for each groundwater cell, and area is computed as per equation P6. $A_{aw} = A_{\max}(1 - S_w)$

Iarea_fn = 2 is when the grain diameter is input for each groundwater cell, and A_{max} is computed as per Lyu equation $A_{\max} = 3.9d^{-1.2}$

Iarea_fn = 3 is when ROG_SIGMA is read ($\rho_w g / \sigma_o$) and A_{aw} is computed as per $A_{aw} = \frac{\rho_w g \phi}{\sigma_o} \int_{S_w}^{1} h \quad dS_w$. Note that this is not yet available in the code.

Iarea_fn = 4 is when x2, x2 and x0 are input for each groundwater cell, and area is computed as per equation P4. $A_{aw} = x_2 S_w^2 + x_1 S_w + x_0$

Iarea_fn = 5 is when tabular input for the area versus saturation function is provided for each location in the groundwater domain.

Options for the air-water interfacial partition coefficient as a function of the solute concentration for each solute component include:

Ikawi_fn = 1 is when the Langmuir coefficients A and B are read. The Langmuir equation for air-water interface partitioning is $c_{aw} = \frac{A}{1+Bc_w} A_{aw} c_w$

Ikawi_fn = 2 is when the coefficients of Silva et al equation (P9) c_{max} and $K_{L,aw}$ are read, and the following equation is used for the computation $c_{aw} = \frac{c_{\max,aw} K_{L,aw}}{1+K_{L,aw}c_w} A_{aw} c_w$. The Langmuir coefficients are: $A = c_{\max} K_L$ and $B = K_L$

Ikawi_fn = 3 is when the coefficient σ_o / RT and coefficient arrays a_w and b_w are read, and equation (P8) $c_{aw} = \frac{1}{RT} \frac{\sigma_0 b_{aw}}{a_{aw}+c_w} A_{aw} c_w$ is used for calculating a-A-W concentrations using Langmuir coefficients internally computed as: $A = (\sigma_o / RT)(b_w / a_w)$ and $B = 1/a_w$

Ikawi_fn = 4 is when tabular input for the air-water interface partitioning coefficient versus solute concentration function is provided for each solute throughout the groundwater domain.

Note that tabular input can be provided for the area-saturation function, the k_{awi}-concentration function, or both. If both functions use tabular input, they both use the same zone-map to distribute the parameters on the model grid and have the same number of rows of tabular input.

WRITE_GWMASS imasswr — is a flag indicating that the cell-by-cell mass of solutes in the groundwater domain is written to a file and the integer **imasswr** following the flag is the Fortran unit number on which the mass is written. The mass is the total mass in the mobile domain (if dual domain simulations are performed) and includes mass in water, on soil solids (if adsorption is on), and on the air-water interface (if A-W_ADSORB is on). The file format is the same as that for species concentrations and is written when concentrations are written.

MULTIFILE crootname — "MULTIFILE" is a flag indicating that concentration output (for multispecies simulations) will be written on multiple files instead of all species on one file. The entry "crootname" includes the rootname of the concentration output binary file. The species number will be attached to this root name and an extension of .CON will be applied to each file. For a thermal simulation, the word "TMPR" will be attached to the rootname (the extension will remain .CON for compatibility with third party vendor software).

Note that when IHEAT=1, all immobile components species number will be incremented by 1. Also, if CLN is on and if CLN output is written to a separate file, then with "MULTIFILE", the entire filename will be the rootname, followed by the species number, followed by the letters "_CLN" followed by the extension ".CON".

MBEGWUNF—is the unit number for output of flow imbalance information for the groundwater domain.

MBEGWUNT—is the unit number for output of transport mass imbalance information for the groundwater domain.

MBECLNUNF—is the unit number for output of flow imbalance information for the CLN domain.

MBECLNUNT—is the unit number for output of transport mass imbalance information for the CLN domain.

HTCONDW—is the heat conductivity of water.

RHOW—is the density of water.

HTCAPW—is the heat capacity of water.

NUZONES—is the number of soil zones for which tabular input is provided for adsorption functions on the air-water interface. The same zones are used for both tabular input of area-saturation and / or Kaw-concentration functions.

NUTABROWS—is the number of rows of tabular input for the area-saturation and / or Kaw-concentration functions.

IAWIZONMAP—is the air-water interfacial tabular input map. Note that if tabular input is used for either the interface area-saturation relation or the Kaw-concentration relations this map

is read. If tables are used for both relationships, then the same map is used for both functions.

ROG_SIGMA—is the specific gravity of water divided by its air-water interfacial tension.

SIGMA_RT—is the air-water interfacial tension divided by constant R and temperature T.

[AWI_AREA_TAB(SAT, AREA)]—is a row within the table of interfacial area versus saturation. The two entries per row are the saturation (SAT) and the related area (AREA) value for that saturation. This item is repeated "**nutabrows**" times for all the rows of the table, which is then repeated "**nuzones**" times for each soil-type zone.

ICBUND—is the boundary variable. One value is read for every model cell. Usually, these values are read one layer at a time; however, when the XSECTION option is specified, a single two-dimensional variable for the cross section is read. Note that although ICBUND may be read as one or more two-dimensional variables, it is stored internally only as a one-dimensional variable for all nodes in the domain. Note that ICBUND is read only when the inactive domain for transport is different than that for the corresponding flow simulation.

If ICBUND(N) = 0, node N is inactive for transport calculations.

If ICBUND(N) > 0, node N is an active cell for solution to the transport equation.

Note that ICBUND can be inactive for active flow nodes. However, ICBUND cannot be active for a node which is inactive for the corresponding flow simulation.

PRSITY—is the effective transport porosity of the medium.

BULKD—is the bulk density of the porous matrix.

ANGLEX—is the angle between the horizontal x-axis and the outward normal to the face between a node and its connecting nodes.

DL—is the longitudinal dispersivity for an isotropic medium

DT—is the transverse dispersivity for an isotropic medium

DLX—is the x-direction longitudinal dispersivity for an anisotropic medium

DLY—is the y-direction longitudinal dispersivity for an anisotropic medium

DLZ—is the z-direction longitudinal dispersivity for an anisotropic medium

DTXY—is the xy-direction transverse dispersivity for an anisotropic medium and is the transverse dispersivity in the y-direction due to flow in the x-direction (DTXY = DTYX)

DTYZ—is the yz-direction transverse dispersivity for an anisotropic medium and is the transverse dispersivity in the z-direction due to flow in the y-direction (DTYZ = DTZY)

DTXZ—is the xz-direction transverse dispersivity for an anisotropic medium and is the transverse dispersivity in the z-direction due to flow in the x-direction (DTXZ = DTZX)

HTCAPS—is the heat capacity of the soil.

HTCONDS—is the heat conductivity of the soil.

AWAMAX—is the maximum area of the air-water interface for interface adsorption computations when IAREA_FN = 1.

GRAIN_DIA—is the grain diameter in centimeters used for computing maximum area of the air-water interface for interface adsorption computations when IAREA_FN = 2. Note that GRAIN_DIA is read into array AWAMAX and computation of AMAX is done internally.

AWAREA_X2—is the factor x2 for computing area of the air-water interface for interface adsorption computations when IAREA_FN = 4.

AWAREA_X1—is the factor x1 for computing area of the air-water interface for interface adsorption computations when IAREA_FN = 4.

AWAREA_X0—is the factor x0 for computing area of the air-water interface for interface adsorption computations when IAREA_FN = 4.

SOLLIM—is the solubility limit for component ICOMP.

SOLSLOPE—is the equilibrium partitioning coefficient for component ICOMP. The SOLSLOPE allows for supersaturated conditions to exist for any solute species. If a solute precipitates

out fully at the solubility limit then set SOLSLOPE to a very high value, though too high a value can cause truncation issues (a value of 1e6 to 1e10 should be adequate).

NPARENT—is the number of parents to component ICOMP.

JPARENT—is an integer array of size NPARENT, containing the solute species numbers of the parent species to component ICOMP.

STOTIO—is a real array of size NPARENT, containing the stoichiometric coefficient or the mass units of ICOMP generated due to decay of one mass unit of parent JPARENT.

SPTLRCT—is a real array of location dependent stoichiometric coefficients indicating mass units of ICOMP generated due to decay of one mass unit of parent JPARENT. This is provided for every node. First, the value of SPTLRCT is read for all nodes of the first parent component, then for the next, till all NPARENT component stoichiometric coefficients are defined at all GWF cells within the domain. For CLN cells, the SPTLRCT values are read in the CLN package where other transport variables for the CLN domain are also read.

ALANGAW—is the Langmuir coefficient for partitioning of each mobile solute at the air-water interface. The formulation used depends on the value of the flag IKAWI_FN.

BLANGAW—is the Langmuir coefficient for partitioning of each mobile solute at the air-water interface. The formulation used depends on the value of the flag IKAWI_FN.

The values of ALANGAW and BLANGAW that are read have different interpretations depending on the flag IKAWI_FN.

If IKAWI_FN = 1 ALANGAW and BLANGAW are the Langmuir coefficients A and B.

If IKAWI_FN = 2 ALANGAW and BLANGAW are the C_{max} and K_L arrays for use with equation (P9), i.e., $c_{aw} = \frac{c_{\max,aw} K_{L,aw}}{1 + K_{L,aw} c_w} A_{aw} c_w$ and the Langmuir coefficients A and B are computed as $A = C_{max} + K_L$ and $B = K_L$.

If IKAWI_FN = 3 ALANGAW and BLANGAW are respectively, the coefficient arrays a_{aw} and b_{aw} of the Brusseau formulation (equation P7) which is used for air-water partitioning i.e., $K_{aw} = \frac{1}{RT} \frac{\sigma_0 b_{aw}}{a_{aw} + c_w}$. and the Langmuir coefficients A and B are computed as $A = \sigma_0 b_{aw}$

/ a_{aw} /RT and B = 1 / a_{aw}. The term σ_0/RT was read in as a constant previously in data item 1E. Note the input uses array **ALANGAW** for a_{aw} and **BLANGAW** for b_{aw}.

[AWI_KAWI_TAB(CONC, KAWI, ICOMP)]—is a row within the table of Kawi versus concentration for species ICOMP. The two entries per row are the concentration and the related Kawi value for that concentration, for the component under consideration. This item is repeated "**nutabrows**" times for all the rows of the table, which is then repeated "**nuzones**" times for each soil-type zone.

ADSORB—is the adsorption coefficient of a contaminant species.

FLICH—is the Freundlich adsorption isotherm exponent of a contaminant species if IADSORB = 2; or is the Langmuir adsorption isotherm constant for a contaminant species if IADSORB = 3.

ZODRW—is the zero-order decay coefficient in water (concentration/time)

ZODRS—is the zero-order decay coefficient on soil (concentration/time)

ZODRAW—is the zero-order decay coefficient on air-water interface (concentration/time)

FODRW—is the first-order decay coefficient in water (1/time)

FODRS—is the first-order decay coefficient on soil (1/time)

FODRAW—is the first-order decay coefficient on air-water interface (1/time)

CONC—is the initial concentration of each contaminant species at any location in the domain. For heat transport, the temperature (TMPR) is read in this variable. If transport solution is for solutes and heat, then the mobile component species are read first (from 1 through MCOMP), then the temperature is read next, followed by the immobile component species (from 1 through IMCOMP).

PRESCRIBED CONCENTRATION BOUNDARY PACKAGE INPUT INSTRUCTIONS

Input to the Prescribed Concentration Boundary (PCB) Package is read from the file that has type "PCB" in the Name File. Optional variables are shown in brackets. All variables are free format if the option "FREE" is specified in the Basic Package input file; otherwise, the non-

optional variables have 10-character fields and the optional variables are free format. Note that if temperature is to be prescribed then its entry follows that of all the mobile solute species.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. [PARAMETER NPPCB MXL]

This optional item must start with the word "PARAMETER".

2. MXPCB IPCBCB [Option]

3. [PARNAM PARTYP Parval NLST *[INSTANCES* NUMINST]]

Repeat Item 3 combined with the indicated repetitions of Item 4 NPPCB times. Items 3 and 4 are not read if NPPCB is negative or 0.

If PARNAM is to be a time-varying parameter, the keyword "INSTANCES" and a value for NUMINST must be entered.

4a. [INSTNAM]

4b. [Layer Row Column Species_No Pconcfact [xyz]]

Omit Item 4b if unstructured grid is used (i.e., if IUNSTR = 1)

4c. Node Species_No Pconcfact [xyz]

Omit Item 4c if structured grid is used (i.e., if IUNSTR = 0)

After each Item 3 for which the keyword "INSTANCES" is not entered, read Item 4b or 4c and not Item 4a.

After each Item 3 for which the keyword "INSTANCES" is entered, read Item 4a and Item 4b or 4c for each instance.

NLST repetitions of Item 4b or 4c are required; they are read by subroutine ULSTRD. (SFAC of the ULSTRD utility subroutine applies to Pconcfact). The NLST repetitions of Item 4b or 4c follow each repetition of Item 4a when PARNAM is time varying.

FOR EACH STRESS PERIOD

5. ITMP NP

6a. Layer Row Column iSpecies_No Conc [xyz]
Omit Item 6a if unstructured grid is used (i.e., if IUNSTR = 1)

6b. Node iSpecies_No Conc [xyz]
Omit Item 6b if structured grid is used (i.e., if IUNSTR = 0)

ITMP repetitions of Item 6a or 6b are read by subroutine ULSTRD if ITMP > 0. (SFAC of the ULSTRD utility subroutine applies to Cond.) Item 6a or 6b is not read if ITMP is negative or 0.

7. [Pname [Iname]]
(Item 7 is repeated NP times. Item 7 is not read if NP is negative or 0. Iname is read if Pname is a time-varying parameter.)

Explanation of Variables Read by the PCB Package

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPPCB—is the number of prescribed concentration parameters.

MXL—is the maximum number of prescribed concentration cells that will be defined using parameters.

MXPCB—is the maximum number of prescribed concentration cells in use during any stress period, including those that are defined using parameters.

IPCBCB—is a flag and a unit number.

If **IPCBCB > 0**, mass flux at each prescribed concentration boundary cell for the respective species will be written to this unit number when “SAVE BUDGET” or a nonzero value for ICBCFL is specified in Output Control.

If **IPCBCB = 0**, mass flux at prescribed concentration boundaries will not be written.

If **IPCBCB < 0**, mass flux at each prescribed concentration boundary cell for the respective species will be written to the listing file when “SAVE BUDGET” or a non-zero value for ICBCFL is specified in Output Control.

Option—is an optional list of character values.

“**AUXILIARY abc**” or “**AUX abc**”—defines an auxiliary variable, named “abc”, which will be read for each prescribed concentration condition as part of Items 4 and 6. Up to 20 variables can be specified, each of which must be preceded by “AUXILIARY” or “AUX.” These variables will not be used by the Groundwater Transport Process, but they will be available for use by other processes. The auxiliary variable values will be read after the Conc variable. “NOPRINT”—specifies that lists of PCBs will not be written to the Listing File.

PARNAM—is the name of a parameter. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter. For the PCB Package, the only allowed parameter type is PCB, which defines values of the prescribed concentration value.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NLST—is the number of prescribed concentration boundary conditions (one for each species that is prescribed at every PCB node) in a non-time-varying parameter. For a time-varying parameter, NLST is the number of prescribed concentration boundary conditions in each instance.

INSTANCES—is an optional keyword that designates a parameter as time varying. The keyword is not case sensitive; that is, any combination of the same characters with different case

can be used. If ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, PARNAM is non-time-varying and NUMINST should not be present.

NUMINST—is the number of instances for a time-varying parameter, where each instance is a list of river reaches and associated properties. If the keyword ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, NUMINST should not be present.

INSTNAM—is the name of an instance associated with the parameter named in the corresponding Item 3. The instance name can be 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent. Instance names must be unique for a parameter, but instance names may be reused for different parameters.

Layer—is the layer number of the cell containing the prescribed concentration boundary.

Row—is the row number of the cell containing the prescribed concentration boundary.

Column—is the column number of the cell containing the prescribed concentration boundary.

Node—is the node number of the model cell that contains the prescribed concentration boundary.

iSpecies_No—is the species number of the prescribed concentration boundary. Note that temperature is the species number after all mobile species are counted.

Concfact—is the factor used to calculate the concentration from the parameter value. The conductance is the product of Concfact and the parameter value.

[xyz]—represents the values of the auxiliary variables for a PCB that have been defined in Item 2. The values of auxiliary variables must be present in each repetition of Items 4 and 6 if they are defined in Item 2. The values must be specified in the order used to define the variables in Item 2.

ITMP—is a flag and a counter.

If **ITMP < 0**, non-parameter PCB data from the last stress period will be reused.

If **ITMP ≥ 0**, ITMP will be the number of non-parameter PCB conditions read for the current stress period.

NP—is the number of parameters in use in the current stress period.

Conc (or Temperature)—is the prescribed concentration value for species (iSpecies_No) at the boundary.

Pname—is the name of a parameter that is being used in the current stress period. NP parameter names will be read.

Iname—is an instance name that is read only if Pname is a time-varying parameter. Multiple instances of the same parameter are not allowed in a stress period.

DENSITY DRIVEN FLOW (DDF) PACKAGE INPUT INSTRUCTIONS

Input to the Density Driven Flow (DDF) Package is read from the file that has type "DDF" in the Name File. All single valued variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format.

For density driven flow, the boundary files for CHD and GHB are also modified. The modification is to allow options for input of different “head” values. Specifically, the user can input the hydraulic head or the potential head (defined above). Options govern which head is defined and conversion is done internally by the code as needed.

FOR EACH SIMULATION

0. [**#Text**]
   Item 0 is optional—“#” must be in column 1. Item 0 can be repeated multiple times.

1. **RHOFRESH, RHOSTD, CSTD, ITHICKAV, IMPH**

Explanation of Variables Read by the DDF Package

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The “#” character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

RHOFRESH—is the density of freshwater

RHOSTD—is the density of standard solution

CSTD—is the concentration of standard solution

ITHICKAV—is a flag indicating if thickness weighted averaging should be used for the density term

ITHICKAV = 0 if arithmetic averaging is used.

ITHICKAV = 1 if thickness weighting averaging is used.

IMPHDD—is a flag indicating if the hydraulic head term in the density formulation is to be treated implicitly or explicitly

IMPHDD = 0 if treatment of the head term is explicit (on the right-hand side vector) maintaining symmetry of the matrix.

IMPHDD = 1 if treatment of the head term is implicit (on the left-hand side matrix) thus creating an asymmetric matrix.

MATRIX DIFFUSION TRANSPORT (MDT) PACKAGE INPUT INSTRUCTIONS

Input for the Matrix Diffusion Transport (MDT) Package is read from the file that is type "MDT" in the Name File. The MDT Package input instructions include flags, indices, transport related parameters and initial conditions for solution to transport of contaminants in a steady-state or transient flow field, for the matrix domain of the dual porosity system. The MDT package functions in a similar manner to the DPT package in that it addresses matrix diffusion in a simulation. The MDT package uses a semi-analytical solution for solute mass evolution within the matrix domain and therefore provides greater accuracy than the DPT formulation which solves for this diffusion numerically, with only one node representing the entire matrix domain. Since concentration differences in the matrix domain can be large within small distances, the DPT formulation with just one average matrix concentration may not be sufficient in many cases to accurately depict the transport of solutes where the semi-analytical solution is required. The MDT package differs from the DPT package in several other ways. Specifically, simplifications and assumptions to the semi-analytical solution are required as listed below:

- Zeroth order decay is not considered within the matrix. Only first order decay is allowed.
- Nonlinear adsorption is not considered within the matrix. Only linear adsorption is allowed.
- Branched chain decay is not considered within the matrix. Only straight chains are allowed.
- Decay is assumed to only occur in the aqueous phase; however, decay in the matrix domain can be simulated with the same decay coefficient as in water if the decay coefficient is multiplied by the matrix retardation factor for the solute.
- For transient flow conditions, the matrix is assumed to be at steady-state and there is no flow of water between the fracture domain and the matrix domain. Therefore, it is assumed that solutes move into the matrix domain by diffusion only, even in transient flow situations.
- For transient flow conditions, all the storage term is attributed to the fracture domain and none to the matrix domain. This is because of the assumption of no transfer of water between the matrix and fracture domains. In certain situations, the opposite may be the case where fractures provide the flow and little storage, while the matrix provides most of the storage of the domain with water flowing between matrix and fracture under transient flow conditions.
- The saturation of the matrix is assumed to be unity and unchanged throughout the simulation.

Matrix Diffusion Transport Package Input Instructions Note

Input for the mobile (fracture) domain is supplied with the BCT package. The input for MDT is read in a free format. Also note that only UNSRUCTURED input formats are available for the MDT package, even if the rest of the problem was set up as a STRUCTURED finite-difference system.

The flow field for transport is supplied by an associated flow simulation. The hydraulic conductivity supplied for the flow field represents the bulk (fracture plus matrix) material property unless an option FRAKH is set, which indicates that the hydraulic conductivity supplied by the BCF or LPF packages represents the property of the fracture domain only. The MDT package cannot be used with the dual porosity flow (DPF) package, for transient flow conditions.

FOR EACH SIMULATION

1. **IMDTCB IMDTCF** [**OPTIONS**]

   These variables are free format if the option “FREE” is specified in the Basic Flow Package input file; otherwise, the variables all have 10-character fields.

   The rest of the file contains arrays of dual porosity transport properties. The variables needed for each cell depend on the transport options that are selected. Unneeded variables must be omitted. The required variables are read for all layers before reading the next variable. Note that there may be a different number of nodes per layer (NDSLAY) for an unstructured grid.

2. **[MDFLAG(NDSLAY)]** – U1DINT. Read one array for each layer.

   If IDPF is zero (flow solution was not dual porosity) then read item 3.

3. **[VOLFRACMD(NDSLAY)]** – U1DINT. Read one array for each layer.

4. **[PORMD(NDSLAY)]** – U1DREL. Read one array for each layer.

5. **[RHOBMD(NDSLAY)]** – U1DREL. Read one array for each layer.

6. **[DIFFLENMD(NDSLAY)]** – U1DREL. Read one array for each layer.

7. **[TORTMD(NDSLAY)]** – U1DREL. Read one array for each layer.

Items 8 – 13 are read for the first component, followed by the next, till all MCOMP species components are read.

8. **[KDMD(NDSLAY,ICOMP)]** – U1DREL. Read one array for each layer.

9. **[DECAYMD(NDSLAY,ICOMP)]** – U1DREL Read one array for each layer

10. **[YIELDMD(NDSLAY,ICOMP)]** – U1DREL Read one array for each layer

11. **[DIFFMD(NDSLAY,ICOMP)]** – U1DREL. Read one array for each layer.

Items 12 – 13 (the concentration integrals AIOLD1MD and AIOLD2MD) are read only if TSHIFTMD OPTION is used. Otherwise, the coefficients are internally set to zero to

denote that the concentration in the matrix domain is zero at the start of the simulation.

12. **[AIOLD1MD(NDSLAY,ICOMP)]** – U1DREL Read one array for each layer

13. **[AIOLD2MD(NDSLAY,ICOMP)]** – U1DREL. Read one array for each layer.

Explanation of Variables Read by the MDT Package:

IMDTCB—is a flag and a unit number.

If **IMDTCB > 0**, cell-by-cell mass flux terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control. The term that is saved is the mass flux between the fracture and the matrix for every cell.

If **IMDTCB = 0**, cell-by-cell mass flux terms will not be written.

If **IMDTCB < 0**, cell-by-cell mass flux for will be written in the listing file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control. The term that is written is the mass flux between the fracture and the matrix for every cell.

IMDTCF—is a flag and a unit number.

If **IMDTCF > 0**, the matrix coefficients ai1 and ai2 will be written to this unit number in a binary format when "SAVE CONC" is included (or a nonzero value of the flag ICONSV is specified) in Output Control.

If **IMDTCF = 0**, immobile domain concentrations will not be saved.

If **IMDTCF < 0**, immobile domain concentrations will be written to the listing file when the “PRINT CONC” is included (or a nonzero value of the flag ICONSV is specified) in Output Control.

OPTIONS—are optional keywords that activate options. Note that these options are required only if the flow simulation is also not dual porosity and indicates how to handle the flow simulation parameters.

FRAHK—indicates that the hydraulic conductivity and storage terms (for transient simulations) which are input are only for the fracture (mobile) domain. Otherwise, it is assumed that the hydraulic conductivity and storage input for the flow simulation are effective hydraulic conductivity and storage terms for the medium, representative of the entire volume.

FRADARCY—indicates that the Darcy flux should be computed only for the fracture domain by use of this hydraulic conductivity value. Thus, the input hydraulic conductivity is divided by the fracture volume fraction. Also, the storage terms (for transient simulations) which are input are only for the fracture (mobile) domain.

TSHIFTMD tshift —the keyword **TSHIFTMD** indicates that the MODFLOW start time (t = 0) is not the starting time of matrix diffusion, and the subsequent real variable **tshift** is the value of time already elapsed since matrix diffusion began. Note that if **TSHIFTMD** is read, then the coefficients AIOLD1MD and AIOLD2MD are also input. Otherwise these coefficients are initialized as zero representing a matrix without solutes.

SEPARATE_AI2 iunitAI2 —the keyword **SEPARATE_AI2** indicates that the output of AI2 in the binary output file for matrix domain average concenrations is put in a separate binary file from AI1. Note that AI2 is 0 if the fmag MDFLAG = 2 for when matrix diffusion occurs only for a matrix emnedded within the cell. Note that a file should also be opened in the NAME file of the simulation to save the AI2 arrays with the same unit number as **iunitAI2**.

MULTIFILE_MD crootname_md — "MULTIFILE_MD" is a flag indicating that AI1 and AI2 output (for multispecies simulations) will be written on multiple files instead of all species on one file. The entry "**crootname_md**" includes the rootname of the concentration output binary file. The species number will be attached to this root name and an extension of AI1 will be applied to each file. If SEPARATE_AI2 is written, then the extension of AI2 will be applied to each file.

MDFLAG—is the matrix diffusion type flag at any location. This flag gives options at each cell on how the matrix diffusion is treated. One value is read for every model cell. Usually, these values are read one layer at a time; however, when the XSECTION option is specified, a single two-dimensional variable for the cross section is read.

If **MDFLAG (N) = 0**, cell N is inactive in the matrix domain (either the cell itself is inactive or the matrix domain does not exist at this cell).

If **MDFLAG(N) = 1**, cell N is active in the matrix domain with matrix diffusion occurring at the bottom of the cell.

If **MDFLAG(N) = 2**, cell N is active in the matrix domain with matrix diffusion occurring embedded within the cell.

If **MDFLAG(N) = 3**, cell N is active in the matrix domain with matrix diffusion occurring at the top of the cell.

If **MDFLAG(N) = 4**, cell N is active in the matrix domain with matrix diffusion occurring at both the top and bottom of the cell.

If **MDFLAG(N) = 5**, cell N is active in the matrix domain with matrix diffusion occurring at the bottom and embedded within the cell.

If **MDFLAG(N) = 6**, cell N is active in the matrix domain with matrix diffusion occurring at the top and embedded within the cell.

If **MDFLAG(N) = 7**, cell N is active in the matrix domain with matrix diffusion occurring at the top, bottom and embedded within the cell.

Note that MDFLAG can be inactive for active flow nodes. However, MDFLAG cannot be active for a node which is inactive for the corresponding flow and transport simulation.

VOLFRACMD—is the mobile fraction at any location, i.e., the fraction of the total space that is occupied by the fracture/high permeability domain. Note that this is the same as PHIF in DPT.

PORMD—is the effective transport porosity within the matrix domain at any location.

RHOBMD—is the dry bulk density of the porous matrix of the matrix domain at any location.

DIFFLENMD—is the diffusion length for diffusive transport within the matrix domain at any location (only used for embedded heterogeneity).

TORTMD—is the tortuosity of the matrix domain at any location.

KDMD—is the adsorption coefficient (K_d) of a contaminant species in the immobile domain at any location.

DECAYMD—is the first-order decay coefficient in water and on soil (1/time) in the matrix domain at any location.

YIELDMD—is the yield coefficient for chain decay at any location. The value indicates mass of species generated by decay of the parent component. Note that component 1 is not a daughter product for any reaction and therefore the yield coefficient should be set to zero (as it is still read for all components).

DIFFMD—is the diffusion coefficient of each species component within the matrix domain at any location.

AIOLD1MD—is the concentration integral (equation 8) of each species in an element associated with matrix diffusion into an infinite acting adjacent aquitard (MDFLAG = 1, 3, 4, 5, 6, or 7). This value is used to restart a simulation with prior matrix diffusion.

AIOLD2MD—is the concentration integral (equation 8) of each species in an element associated with matrix diffusion in low permeability zones that are embedded in the volume element (MDFLAG = 2, 5, 6, or 7). This value is used to restart a simulation with prior matrix diffusion.

DUAL POROSITY TRANSPORT (DPT) PACKAGE INPUT INSTRUCTIONS

Input for the Dual Porosity Transport (DPT) Package is read from the file that is type "DPT" in the Name File. The DPT Package input instructions include flags, indices, transport related parameters and initial conditions for solution to transport of contaminants in a steady-state or transient flow field, for the immobile (matrix) domain of the dual porosity system. Input for the mobile (fracture) domain is supplied with the BCT package. The input for DPT is read in a free format. Also note that only UNSRUCTURED input formats are available for the DPT package, even if the rest of the problem was set up as a STRUCTURED finite-difference system.

The flow field for transport is supplied by an associated flow simulation. The hydraulic conductivity supplied for the flow field represents the bulk (fracture plus matrix) material property

unless an option FRAKH is set, which indicates that the hydraulic conductivity supplied by the BCF or LPF packages represents the property of the fracture domain only.

The DPT package may be used with or without the dual porosity flow (DPF) package, for transient flow conditions (note that for steady-state flow conditions, there is no change in fluid volume storage and thus the DPF package is not required). ***For transient flow cases, appropriate physical behavior of the system can be simulated only if the effective porosity in each domain (input via the BCT and DPT package) is greater than or equal to the specific yield (drainable porosity) of that domain (input via the BCF/LPF and DPF package)***. Thus, if the DPF package is not invoked for a DPT simulation with a transient flow field, the storage terms are appropriately checked for consistency. If the flow simulation input (in the BCF or LPF file) is considered for the fracture domain only (using the option FRAKH), then the hydraulic conductivity and storage terms are scaled by the fracture porosity to obtain the governing equation for the entire domain. If, however, the flow simulation variables are considered to represent the total medium (fracture plus matrix), a check is performed to note if the porosity of the fracture domain (input via the BCT package) is larger than the associated specific yield (which is attributed only to the mobile domain for consistency). If not, the porosity of the fracture domain is made equal to the specific yield scaled for the fraction of the volume that represents the fracture domain. A warning message is provided in the output listing file if this is done.

As in the BCT package, inputs for the various options used in the DPT package are highlighted. Options for solubility and chain decay are the same as for the BCT package. Heat transport simulation can also include the immobile domain. **The air-water interface adsorption** routines that are included in the BCT package are also available for the immobile domain of a dual domain simulation via the DPT package. This feature is meant to accommodate PFAS and related compounds that are surfactant-like and may be held back on the air-water interface in the vadose zone. The option is meant to be used with simulating Richards' equation for saturated / unsaturated flow. PFAS compounds may also have an impact on the air-water capillarity thus affecting the moisture retention curves. Furthermore, PFAS solutions can have a wide range of viscosities that may affect flow. These impacts may be included by adjusting the van Genuchten parameters and the viscosity in a time-lagged manner but are neglected in the code for now. The air-water interface adsorption routines in the immobile domain have independent input from

that of the mobile domain and therefore, a user can have this feature only in the mobile domain, only in the immobile domain, or both for a dual domain simulation.

FOR EACH SIMULATION

1a. **IDPTCB IDPTCON ICBNDIMFLG IADSORBIM IDISPIM IZODIM IFODIM** [**OPTIONS**]

These seven variables are free format if the option "FREE" is specified in the Basic Flow Package input file; otherwise, the variables all have 10-character fields.

1b. NAZONESIM NATABROWSIM – Format free. The variable **nazones** represents the number of soil zones, and the variable **natabrows** indicates the number of rows of tabular input to define the function for the air-water interface area, or the air-water interface partitioning coefficient, or both.

Read item 1b only if AW_ADSORBIM option in item 1a above is used and either flag IAREA_FNIM = 5 or IKAWI_FNIM = 4 (i.e., tabular input is used for the area or Kaw functions).

1c. [IAWIZONMAPIM (NODES)] -- U1DINT. Read one integer array for all groundwater nodes.

Read item 1c only if AW_ADSORBIM option in item 1a above is used and either flag IAREA_FNIM = 5 or IKAWI_FNIM = 4 (i.e., tabular input is used for the area or Kaw functions).

1d. ROG_SIGMAIM

Read item 1d only if AW_ADSORBIM option in item 1a above is used and the flag IAREA_FNIM = 4.

1e. SIGMA_RTIM

Read item 1e only if AW_ADSORBIM option in item 1a above is used and the flag IKAWI_FNIM = 3.

1f. [AWI_AREA_TABIM **(SAT, AREA)]** – One row for each of the "**natabrowsim**" of a table, which is then repeated "**nazonesim**" times for each soil zone in the catalogue.

Read item 1f only if AW_ADSORBIM option in item 1a above is used and flag IAREA_FNIM = 5. (i.e., tabular input is used for the area-saturation function). Item 1g has natabrowsim times nazonesim the number of entries where each entry is the area for a given saturation in the saturation – area function.

The rest of the file contains arrays of dual porosity transport properties. The variables needed for each cell depend on the transport options that are selected. Unneeded variables must be omitted. The required variables are read for all layers before reading the next variable. Note that there may be different number of nodes per layer (NDSLAY) for an unstructured grid.

If ICBNDIMFLG is not zero then read item 2.

2. **[ICBUNDIM(NDSLAY)]** – U1DINT. Read one array for each layer.

   If IDPF is zero (flow solution was not dual porosity) then read item 3.

3. **[PHIF(NDSLAY)]** – U1DINT. Read one array for each layer.

4. **[PRSITYIM(NDSLAY)]** – U1DREL. Read one array for each layer.

   If IADSORBIM is not zero then read item 5.

5. **[BULKDIM(NDSLAY)]** – U1DREL. Read one array for each layer.

   If IDPF is not zero (flow solution was dual porosity) then read item 6.

6. **[DLIM(NDSLAY)]** – U1DREL. Read one array for each layer.

7. **[DDTR(NDSLAY)]** – U1DREL. Read one array for each layer.

   If IDPF is zero (flow solution was not dual porosity) and the optional keyword INPUTSAT was read on item 1, then read item 8.

8. **[SIM(NDSLAY)]** – U1DREL. Read one array for each layer.

If IHEAT is equal to ONE then read the following items H1 and H2.

H1. [HTCAPSIM(NDSLAY,MCOMPT)] – U1DREL. Read one array for each layer till all layers are read. Note that the soil heat capacity is actually read in array ADSORB as the

adsorption term in solute transport is equivalent to the soil heat storage of the energy equation.

A1. AWAMAXIM(NDSLAY) – U1DREL. Read one array for each layer till all layers are read.

Read item A2, A3 and A4 if IAREA_FNIM is 2.

A2. AWAREA_X2IM(NDSLAY) – U1DREL. Read one array for for each layer till all layers are read.

A3. AWAREA_X1IM(NDSLAY) – U1DREL. Read one array for for each layer till all layers are read.

A4. AWAREA_X0IM(NDSLAY) – U1DREL. Read one array for for each layer till all layers are read.

Read item A5 if IAREA_FNIM is 3.

A5. GRAIN_DIAIM(NDSLAY) – U1DREL. Read one array for each layer till all layers are read.

Items C and 9 – 15 are read for the first component, followed by the next, till all MCOMP contaminant species are read.

Read item C only if the SPATIALREACT option is turned on in the BCT input file.

C. [SPTLRCTIM(NDSLAY,ICOMP,MCOMP)] – U1DREL. Read one array for each layer till all layers are read, then for all parent components of this component ICOMP including the component itself (with a value of zero).

If AW_ADSORBIM option is on, then read the following items A6, A7 and A8.

A6. [ALANGAWIM(NDSLAY,ICOMP)] – U1DREL. Read one array for each layer till all layers are read.

A7. [BLANGAWIM(NDSLAY,ICOMP)] – U1DREL. Read one array for each layer till all layers are read.

A8. **[AWI_KAWI_TABIM(CONC, KAWI, ICOMP)]** – One row for each of the "**nutabrowsim**" of a table, which is then repeated "**nuzonesim**" times for each soil zone in the catalogue.

Read item A8 only if AW_ADSORBIM option in item 1a above is used and flag IKAWI_FNIM = 4. (i.e., tabular input is used for the Kaw-Concentration function). Item A8 has nutabrowsim times nuzonesim the number of entries where each entry is the adsorption coefficient for a given concentration of this solute in the concentration – K_{awi} function.

If IADSORBIM is not zero then read item 9.

9. **[ADSORBIM(NDSLAY,ICOMP)]** – U1DREL. Read one array for each layer.

   If IADSORBIM is two or three then read item 10.

10. **[FLICHIM(NDSLAY,ICOMP)]** – U1DREL. Read one array for each layer.

    If IZODIM is one or three or four, then read item 11.

11. **[ZODRWIM(NDSLAY,ICOMP)]** – U1DREL Read one array for each layer

    If IADSORBIM is not zero and IZODIM is two or three or four, then read item 12.

12. **[ZODRSIM(NDSLAY,ICOMP)]** – U1DREL Read one array for each layer

    If IAW_ADSORBIM is not zero and IZODIM is 4, then read item 12a.

12a. **[ZODRAWIM(NDSLAY,ICOMP)]** – U1DREL Read one array for each layer

    If IFODIM is one or three or four, then read item 13.

13. **[FODRWIM(NDSLAY,ICOMP)]** – U1DREL Read one array for each layer

    If IADSORBIM is not zero and IFODIM is two or three or four, then read item 14.

14. **[FODRSIM(NDSLAY,ICOMP)]** – U1DREL Read one array for each layer

    If IAW_ADSORBIM is not zero and IFODIM is 4, then read item 14a.

14a. **[FODRAWIM(NDSLAY,ICOMP)]** – U1DREL Read one array for each layer

15. **[CONC(NDSLAY,ICOMP)]** – U1DREL. Read one array for each layer.

Explanation of Variables Read by the DPT Package

IDPTCB—is a flag and a unit number.

If **IDPTCB > 0**, cell-by-cell mass flux terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control. The terms that are saved are mass storage, mass flux from constant-concentration nodes, and mass flux between adjacent cells.

If **IBDPTCB = 0**, cell-by-cell mass flux terms will not be written.

If **IDPTCB < 0**, cell-by-cell mass flux for constant-concentration cells will be written in the listing file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control. Cell-by-cell mass flux to storage and between adjacent cells will not be written to any file.

IDPTCON—is a flag and a unit number.

If **IDPTCON > 0**, immobile domain concentrations will be written to this unit number in a binary format when "SAVE CONC" or a nonzero value and ISPCFL is specified in Output Control.

If **IDPTCON = 0**, immobile domain concentrations will not be saved.

If **IDPTCON < 0**, immobile domain concentrations will be written to the listing file.

ICBNDIMFLG—is a flag that determines if the active domain for the immobile (matrix) domain for transport is the same as that for the mobile (fracture) domain for transport.

If **ICBNDIMFLG = 0**, the active domain for immobile domain is not the same as for the mobile domain and is read.

If **ICBNDIMFLG = 1**, the active domain for the immobile domain is the same as IBOUND for the mobile domain for transport and the transport IBOUND array does not need to be read but is set from that of flow.

IADSORBIM—is an adsorption flag.

If **IADSORBIM = 0**, then adsorption is not simulated.

If **IADSORBIM = 1,** then linear adsorption is simulated.

If **IADSORBIM = 2**, then Freundlich adsorption is simulated.

If **IADSORBIM = 3**, then Langmuir adsorption is simulated.

IDISPIM—is a flag indicating the dispersion formula used in the model

If **IDISPIM = 0**, then dispersion is not simulated.

If **IDISPIM = 1**, then dispersion is simulated.

IZODIM—is a flag indicating if zero order decay is simulated

If **IZODIM = 0**, then zero order decay is not simulated.

If **IZODIM = 1**, then zero order decay is included in water.

If **IZODIM = 2**, then zero order decay is included on soil if there is adsorption.

If **IZODIM = 3**, then zero order decay is included in water and on soil if there is adsorption.

If IZODIM = 4, then zero order decay is included on the air-water interface if there is adsorption onto the air-water interface, along with zero order decay in water and on soil. Note that if zero order decay does not occur in any of the phases, the related coefficient can be set to zero. If there is an air-water interface, with no zero order decay on the air-water interface, the other **IZODIM** options may be used.

IFODIM—is a flag indicating if first order decay is simulated

If **IFODIM = 0**, then first order decay is not simulated.

If **IFODIM = 1**, then first order decay is included in water.

If **IFODIM = 2**, then first order decay is included on soil if there is adsorption.

If **IFODIM = 3**, then first order decay is included in water and on soil if there is adsorption.

If IFODIM = 4, then first order decay is included on the air-water interface if there is adsorption onto the air-water interface, along with first order decay in water and on soil. Note that if first order decay does not occur in any of the phases, the related coefficient can be set to zero. If there is an air-water interface, with no first order decay on the air-water interface, the other **IFODIM** options may be used.

OPTIONS—are optional keywords that activate options. Note that these options are required only if the flow simulation is also not dual porosity and indicates otherwise, how to handle the flow simulation parameters.

FRAHK—indicates that the hydraulic conductivity and storage terms (for transient simulations) which are input are only for the fracture (mobile) domain. Otherwise, it is assumed that the hydraulic conductivity and storage input for the flow simulation are effective hydraulic conductivity and storage terms for the medium, representative of the entire volume.

MOBILESAT—the optional keyword MOBILESAT indicates that the immobile domain saturation will be set equal to the initial mobile domain saturation. Otherwise, the immobile domain saturation is set to unity. Note that for transport in a transient flow-field, the immobile domain saturation is not varied through time to maintain mass balance of flow, since no water exchange is assumed between the domains.

INPUTSAT—the optional keyword INPUTSAT indicates that the immobile domain saturation will be input in this dataset. Otherwise, the immobile domain saturation will be set to unity. Note that for transport in a transient flow-field, the immobile domain saturation is not varied through time to maintain mass balance of flow, since no water exchange is assumed between the domains.

A-W_ADSORBIM iarea_fn ikawi_fn— The keyword **A-W_ADSORBIM** indicates that air-water interface adsorption will be simulated with transport. The flags **iarea_fnim** and **ikawi_fnim** indicate input options for the area v. saturation function, and for the air-water interface partition coefficient Kawi v. concentration function respectively. Options for the area as a function of interfacial saturation include:

Iarea_fnim = 1 is when A_{max} is input for each groundwater cell, and area is computed as per equation P6. $A_{aw} = A_{\max}(1 - S_w)$

Iarea_fnim = 2 is when the grain diameter is input for each groundwater cell, and A_{max} is computed as per Lyu equation $A_{\max} = 3.9d^{-1.2}$

Iarea_fnim = 3 is when ROG_SIGMA is read ($\rho_w g / \sigma_o$) and A_{max} is computed as per $A_{max} = \frac{\rho_w g \phi}{\sigma_o}$

Iarea_fnim = 4 is when x2, x2 and x0 are input for each groundwater cell, and area is computed as per equation P4. $A_{aw} = x_2 S_w^2 + x_1 S_w + x_0$

Iarea_fnim = 5 is when tabular input for the area versus saturation function is provided for each location in the groundwater domain.

Options for the air-water interfacial partition coefficient as a function of the solute concentration for each solute component include:

Ikawi_fnim = 1 is when the Langmuir coefficients A and B are read. The Langmuir equation for air-water interface partitioning is $c_{aw} = \frac{A}{1 + Bc_w} A_{aw} c_w$

Ikawi_fnim = 2 is when the coefficients of Silva et al equation (P11) c_{max} and $K_{L,aw}$ are read, and the Langmuir coefficients are computed as: $A = c_{\max} K_L$ and $B = K_L$

Ikawi_fnim = 3 is when the coefficient σ_o / RT and coefficient arrays a_w and b_w are read, and the Langmuir coefficients are computed as: $A = (\sigma_o / RT)(b_w / a_w)$ and $B = 1 / a_w$

Ikawi_fnim = 4 is when tabular input for the air-water interface partitioning coefficient versus solute concentration function is provided for each solute throughout the groundwater domain.

NUZONESIM—is the number of soil zones for which tabular input is provided. The same zones are used for both tabular input of area-saturation or Kaw-concentration functions.

NUTABROWSIM—is the number of rows of tabular input for the area-saturation or Kaw-concentration functions.

IAWIZONMAPIM—is the air-water interfacial tabular input map. Note that if tabular input is used for either the interface area-saturation relation or the Kaw-concentration relations this map

is read. If tables are used for both relationships, then the same map is used for both functions.

ROG_SIGMAIM—is the specific gravity of water divided by its air-water interfacial tension.

SIGMA_RTIM—is the air-water interfacial tension divided by constant R and temperature T.

[AWI_AREA_TABIM(SAT, AREA)]—is a row within the table of interfacial area versus saturation. The two entries per row are the saturation (SAT) and the related area (AREA) value for that saturation. This item is repeated "**nutabrows**" times for all the rows of the table, which is then repeated "**nuzones**" times for each soil-type zone.

ICBUNDIM—is the boundary variable. One value is read for every model cell. Usually, these values are read one layer at a time; however, when the XSECTION option is specified, a single two-dimensional variable for the cross section is read. Note that although ICBUNDIM may be read as one or more two-dimensional variables, it is stored internally only as a one-dimensional variable for all nodes in the domain. Note that ICBUNDIM is read only when inactive sections of the immobile domain are different from the corresponding inactive sections of the mobile domain.

If **ICBUNDIM(N) = 0**, cell N is inactive in the immobile domain (either the cell itself is inactive or the immobile domain does not exist at this cell).

If **ICBUNDIM(N) > 0**, cell N is active in the immobile domain.

Note that ICBUND can be inactive for active flow nodes. However, ICBUND cannot be active for a node which is inactive for the corresponding flow simulation.

PHIF—is the mobile fraction. i.e., the fraction of the total space that is occupied by the mobile domain.

PRSITYIM—is the effective transport porosity of the immobile domain.

BULKDIM—is the bulk density of the porous matrix of the immobile domain.

DLIM—is the longitudinal dispersivity coefficient for transport between mobile and immobile domains when flow is also dual porosity.

DDTR—is the mass transfer coefficient for diffusive transport between mobile and immobile domains.

SIM—is the saturation in the immobile domain which is input when dual domain flow is not solved.

HTCAPSIM—is the heat capacity of the soil.

AWAMAXIM—is the maximum area of the air-water interface for interface adsorption computations when IAREA_FNIM = 1.

AWAREA_X2IM—is the factor x2 for computing area of the air-water interface for interface adsorption computations when IAREA_FNIM = 2.

AWAREA_X1IM—is the factor x1 for computing area of the air-water interface for interface adsorption computations when IAREA_FNIM = 2.

AWAREA_X0IM—is the factor x0 for computing area of the air-water interface for interface adsorption computations when IAREA_FNIM = 2.

GRAIN_DIAIM—is the grain diameter in centimeters used for computing maximum area of the air-water interface for interface adsorption computations when IAREA_FNIM = 3. Note that GRAIN_DIAIM is read into array AWAMAXIM and computation of AMAXIM is done internally.

SPTLRCTIM—is a real array of location dependent stoichiometric coefficients indicating mass units of ICOMP generated due to decay of one mass unit of parent JPARENT. This is provided for every node if the SPATIALREACT option is invoked in the BCT package. First, the value of SPTLRCT is read for all immobile domain cells of the first parent component, then for the next, till all NPARENT component stoichiometric coefficients are defined at all immobile domain cells within the domain.

ALANGAWIM—is the Langmuir coefficient for partitioning of each mobile solute at the air-water interface. The formulation used depends on the value of the flag IKAWI_FNIM.

BLANGAWIM—is the Langmuir coefficient for partitioning of each mobile solute at the air-water interface. The formulation used depends on the value of the flag IKAWI_FNIM.

The values of ALANGAWIM and BLANGAWIM that are read have different interpretations depending on the flag IKAWI_FNIM.

If IKAWI_FNIM = 1 ALANGAWIM and BLANGAWIM are the Langmuir coefficients A and B.

If IKAWI_FNIM = 2 ALANGAWIM and BLANGAWIM are the C_{max} and K_L arrays and the Langmuir coefficients A and B are computed as $A = C_{max} + K_L$ and $B = K_L$.

If IKAWI_FNIM = 3 BLANGAWIM and ALANGAWIM are the a_{aw} and b_{aw} arrays of the Brusseau formulation and the Langmuir coefficients A and B are computed as $A = \sigma_0 b_{aw} / a_{aw} /RT$ and $B = 1 / a_{aw}$. The term σ_0/RT was read in as a constant previously in data item 1E. Note the input uses array **BLANGAWIM** for a_{aw} and **ALANGAWIM** for b_{aw}.

[AWI_KAWI_TABIM(CONC, KAWI, ICOMP)]—is a row within the table of Kawi versus concentration for species ICOMP. The two entries per row are the concentration and the related Kawi value for that concentration, for the component under consideration. This item is repeated "**nutabrowsim**" times for all the rows of the table, which is then repeated "**nuzonesim**" times for each soil-type zone.

ADSORBIM—is the adsorption coefficient of a contaminant species in the immobile domain.

FLICHIM—is the Freundlich adsorption isotherm exponent of a contaminant species in the immobile domain if IADSORB = 2, or the Langmuir adsorption coefficient if IADSORB = 3.

ZODRWIM—is the zero-order decay coefficient in water (concentration/time) in the immobile domain.

ZODRSIM—is the zero-order decay coefficient on soil (concentration/time) in the immobile domain.

ZODRAWIM—is the zero-order decay coefficient on air-water interface (concentration/time).

FODRWIM—is the first-order decay coefficient in water (1/time) in the immobile domain.

FODRSIM—is the first-order decay coefficient on soil (1/time) in the immobile domain.

FODRAWIM—is the first-order decay coefficient on air-water interface (1/time).

CONCIM—is the initial concentration of each contaminant species at any location in the immobile domain. For heat transport, the temperature (TMPR) is read in this variable. If transport solution is for solutes and heat, then the mobile component species are read first (from 1 through MCOMP), then the temperature is read next, followed by the immobile component species (from 1 through IMCOMP) for the immobile domain.

TRANSIENT IBOUND (TIB) PACKAGE INPUT INSTRUCTIONS

Input to the TIB Package is read from the file that has type "TIB" in the Name File. All single valued variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format. Cell numbers used to identify grid-blocks that turn on or off are input in terms of the global cell number. Note that GWF cells are first numbered followed by CLN cells in the global numbering sequence. For structured GWF grids, the node numbering first follows columns, then rows and finally layers (as is the convention in MODFLOW).

FOR EACH SIMULATION

0. [#Text]

   Item 0 is optional—“#” must be in column 1. Item 0 can be repeated multiple times.

FOR EACH STRESS PERIOD

1. NIB0 NIB1 NIBM1 NICB0 NICB1 NICBM1

Read item 2 only if NIB0 is greater than zero

2. [IBO(NIB0)] -- U1DINT

Read item 3 only if NIB1 is greater than zero

3. IB1 [OPTIONS]

   Note that item 3 is read NIB1 times, one record for each node for which IBOUND is activated.

Read item 4 only if NIBM1 is greater than zero

4. IBM1 [OPTIONS]

   Note that item 4 is read NIBM1 times, one record for each node for which IBOUND is made into a prescribed head.

Read item 5 only if NICB0 is greater than zero

5. [ICBO(NICB0)] -- U1DINT

Read item 6 only if NICB1 is greater than zero

6. ICB1 [**OPTIONS2**]

   Note that item 6 is read NICB1 times, one record for each node for which ICBUND is activated.

Read item 7 only if NICBM1 is greater than zero

7. ICBM1 [**OPTIONS2**]

   Note that item 7 is read NICBM1 times, one record for each node for which ICBUND is made into a prescribed concentration.

Explanation of Variables Read by the TIB Package:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NIB0—is the number of IBOUND values that will be turned to zero in this stress period.

NIB1—is the number of IBOUND values that will be turned to active (one) in this stress period.

NIBM1—is the number of IBOUND values that will be turned to prescribed head (minus one) in this stress period.

NICB0—is the number of ICBUND values that will be turned to zero in this stress period.

NICB1—is the number of ICBUND values that will be turned to active (one) in this stress period.

NICBM1—is the number of ICBUND values that will be turned to prescribed concentration (minus one) in this stress period.

IB0—is the array of cell numbers for which IBOUND values will be set to zero.

IB1—is the cell number for which IBOUND is set to active (one).

OPTIONS — are keywords to indicate how head values will be set for nodes that are activated:

HEAD [hvalue] indicates that the head value is input and the number following the keyword HEAD is the value to be used as the initial head at the given cell.

AVHEAD indicates that the average head of all connected cells that are not inactive, will be used as the initial head at the given cell.

Note that if no options are provided, then the head from the previous stress period will be used at this node which is turned active. If the node was inactive in the previous stress period, an option is required to provide a head value to the cell that is made active or prescribed head, otherwise the simulation will be aborted.

IBM1—is the cell number for which IBOUND is set to prescribed head (minus one). Note that the same options follow IBMI as do IB1 for each cell for which the head will be prescribed in this stress period.

ICB0—is the array of cell numbers for which ICBUND values will be set to zero.

ICB1—is the cell number for which ICBUND is set to active (one). If IBOUND for the cell is 0 (inactive cell), then the simulation will be aborted with an appropriate error message.

OPTIONS2 — are keywords to indicate how concentration values will be set for nodes that are activated:

CONC [cvalue(mcomp)] indicates that the concentration value(s) for each species (a total of mcomp numbers) is input and the number(s) following the keyword CONC is the value to be used as the initial concentration at the given cell.

AVCONC indicates that the average concentration of all connected cells that are not inactive (based on ICBUND), will be used as the initial concentration at the given cell.

Note that if no options are provided, then the concentration from the previous stress period will be used at this node which is turned active. If the node was inactive in the previous stress period, an option is required to provide a concentration value to the cell that is made active or prescribed concentration, otherwise the simulation will be aborted.

ICBM1—is the cell number for which ICBUND is set to prescribed concentration (minus one). Note that the same options follow ICBMI as do ICB1 for each cell for which the concentration will be prescribed in this stress period.

TIME VARYING MATERIALS (TVM2) PACKAGE INPUT INSTRUCTIONS

Input to the Time Varying Materials (TVM) Package is read from the file that is type "TVM" in the Name File. All single-valued variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format. Material properties that can be made transient include horizontal hydraulic conductivity, vertical hydraulic conductivity, speifis storage, specific yield, the dual domain flow transfer coefficient (DDFTR), and the porosity of a transport simulation.

FOR EACH SIMULATION

0. [#Text]

   Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. ITVMPRINT TVMLOGBASEHK TVMLOGBASEVKA TVMLOGBASESS TVMLOGBASESY TVMDDFTR TVMLOGBASEPOR

FOR EACH STRESS PERIOD BOUNDARY (START PERIOD 1, END PERIOD 1, END PERIOD 2, … END PERIOD NPER)

Lines 2 to 7 are specified once for the start of stress period 1, and then repeated once for each stress period in the simulation to specify the property values at the end of each stress period.

2. NTVMHK NTVMVKA NTVMSS NTVMSY NTVMDDFTR NTVMPOR

   Read item 3 only if NTVMHK is greater than zero

3. ITVMHK HKNEW

   Note that item 3 is read NTVMHK times, one record for each node for which HK is to be changed.

   Read item 4 only if NTVMVKA is greater than zero

4. ITVMVKA VKANEW

   Note that item 4 is read NTVMVKA times, one record for each node for which VKA is to be changed.

   Read item 5 only if NTVMSS is greater than zero

5. ITVMSS SSNEW

   Note that item 5 is read NTVMSS times, one record for each node for which SS is to be changed.

   Read item 6 only if NTVMSY is greater than zero

6. ITVMSY SYNEW

   Note that item 6 is read NTVMSY times, one record for each node for which SY is to be changed.

   Read item 7 only if dual porosity flow is simulated and NTVMDDFTR is greater than zero

7. ITVMDDFTR DDFTRNEW

   Note that item 7 is read NTVMDDFTR times, one record for each node for which DDFTR is to be changed.

   Read item 8 only if NTVMPOR is greater than zero.

8. ITVMPOR PORNEW

   Note that item 8 is read NTVMPOR times, one record for each node for which PRSITY is to be changed.

Explanation of Variables Read by the TVM Package

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

ITVMPRINT—a print flag determining how much information the TVM package will print to the listing file. A value of 0 will print no information (except warnings or errors). A value of 1 will print aggregate information about what is read from the TVM input file, and how many changes occurred each time step. A value of 2 will print everything printed when ITVMPRINT=1, as well as printing all individual cell property value interpolation ranges and changes at each time step.

TVMLOGBASEHK—specifies the type of interpolation to use between starting and ending horizontal hydraulic conductivity (HK) property values in each stress period.

If TVMLOGBASEHK = 0, linear interpolation will be used.

If TVMLOGBASEHK > 0, logarithmic interpolation will be used, and TVMLOGBASEHK is taken as the logarithm base.

If TVMLOGBASEHK < 0, a step function will be used, and the value at the start of a stress period will be maintained till the end. The end value is then used at the start of the next stress period.

TVMLOGBASEVKA—specifies the type of interpolation to use between starting and ending vertical hydraulic conductivity (VKA) property values in each stress period.

If TVMLOGBASEVKA = 0, linear interpolation will be used.

If TVMLOGBASEVKA > 0, logarithmic interpolation will be used, and TVMLOGBASEVKA is taken as the logarithm base.

If TVMLOGBASEVKA < 0, a step function will be used, and the value at the start of a stress period will be maintained till the end. The end value is then used at the start of the next stress period.

TVMLOGBASESS—specifies the type of interpolation to use between starting and ending specific storage property values in each stress period.

If TVMLOGBASESS = 0, linear interpolation will be used.

If TVMLOGBASESS > 0, logarithmic interpolation will be used, and TVMLOGBASESS is taken as the logarithm base.
Note that a step function is not supported for specific storage changes as of version 2 of TVM.

TVMLOGBASESY—specifies the type of interpolation to use between starting and ending specific yield property values in each stress period.

If TVMLOGBASESY = 0, linear interpolation will be used.

If TVMLOGBASESY > 0, logarithmic interpolation will be used, and TVMLOGBASESY is taken as the logarithm base.
Note that a step function is not supported for specific yield changes as of version 2 of TVM.

TVMDDFTR—specifies the type of interpolation to use between starting and ending dual domain rate transfer coefficient property values in each stress period.

If TVMDDFTR = 0, linear interpolation will be used.

If TVMDDFTR > 0, logarithmic interpolation will be used, and TVMDDFTR is taken as the logarithm base.

If TVMDDFTR < 0, a step function will be used, and the value at the start of a stress period will be maintained till the end. The end value is then used at the start of the next stress period.

TVMLOGBASEPOR—specifies the type of interpolation to use between starting and ending specific yield property values in each stress period.

If TVMLOGBASEPOR = 0, linear interpolation will be used.

If TVMLOGBASEPOR > 0, logarithmic interpolation will be used, and TVMLOGBASEPOR is taken as the logarithm base. Note that a step function is not supported for porosity changes as of version 2 of TVM.

NTVMHK—is the number of horizontal hydraulic conductivity (HK) values that will be changed at this stress period boundary.

NTVMVKA—is the number of vertical hydraulic conductivity (VKA) values that will be changed at this stress period boundary.

NTVMSS—is the number of Ss values that will be changed at this stress period boundary.

NTVMSY—is the number of Sy values that will be changed at this stress period boundary.

NTVMDDFTR—is the number of DDFTR values that will be changed at this stress period boundary.

NTVMPOR—is the number of porosity values that will be changed at this stress period boundary.

ITVMHK—is the cell number for which horizontal hydraulic conductivity (HK) will be changed.

HKNEW—is the value of horizontal hydraulic conductivity (HK) that should be assigned to the cell at this stress period boundary.

ITVMVKA—is the cell number for which vertical hydraulic conductivity (VKA) will be changed.

VKANEW—is the value of vertical hydraulic conductivity (VKA) that should be assigned to the cell at this stress period boundary. Note that for any cell in a layer with LAYVKA not equal to 0 in the LPF package, this value will represent the ratio of horizontal to vertical hydraulic conductivity instead of vertical hydraulic conductivity.

ITVMSS—is the cell number for which Ss will be changed.

SSNEW—is the value of Ss that should be assigned to the cell at this stress period boundary. If the STORAGECOEFFICIENT option in the LPF package is used, this value represents confined storage coefficient instead of specific storage.

ITVMSY—is the cell number for which Sy will be changed.

SYNEW—is the value of Sy that should be assigned to the cell at this stress period boundary.

ITVMDDFTR—is the cell number for which DDFTR will be changed.

DDFTRNEW—is the value of DDFTR that should be assigned to the cell at this stress period boundary.

ITVMPOR—is the cell number for which porosity will be changed.

PORNEW—is the value of porosity that should be assigned to the cell at this stress period boundary.

RECHARGE (RCH) PACKAGE INPUT INSTRUCTIONS

Input to the Recharge (RCH) Package is read from the file that has type "RCH" in the Name File. All single valued variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format.

Note that the recharge package has been extended from the MODFLOW-2005 version to also include time varying recharge conditions that are prescribed irrespective of stress periods. Thus, recharge events at a smaller temporal scale than stress periods can be applied in a manner similar to time varying heads or fluxes of the Flow and Head Boundary (FHB) package. The time varying recharge conditions are implemented by supplying zonal identification in the RCH input file, with temporally varying recharge supplied as a time series for each zone, via a separate file. ***The final recharge applied to the model is the sum of the recharge values supplied here via stress periods and the time varying recharge values supplied for each zone via the time series file.*** The time varying recharge may be invoked by using the optional keyword RTS to inducate that a recharge time-series will also be read.

Another extension from MODFLOW-2005 is to provide the option for constraining recharge subject to water levels being below a prescribed maximum seepage elevation. This is the non-ponding condition for unconfined recharge. Recharge fluxes adjust (reduce) to observe this constraint if the optional keyword SEEPELEV is used to indicate that seepage-face elevations will also be read.

If transport is simulated with the recharge package, it is assumed by default that concentration in recharge water is zero. If it is required to be non-zero for any species of simulation, the optional keyword CONCENTRATION (or CONC) allows for further input of species that have non-zero concentration, and the concentration array for those species.

FOR EACH SIMULATION

0. [#Text]

   Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. [***PARAMETER*** NPRCH]

   This optional item must start with the word "PARAMETER".

2a. NRCHOP IRCHCB [OPTIONS1]

Item 2b is read only if UNSTRUCTURED option is used and NRCHOP =2

2b. MXNDRCH

Item 2c is read only if option "CONCENTRATION" or "CONC" is used for the simulation

2c. IRCHCONC(MCOMP)

3. [PARNAM PARTYP Parval NCLU [INSTANCES NUMINST]]

   Repeat Item 3 combined with the indicated repetitions of Item 4 NPRCH times. Items 3 and 4 are not read if NPRCH is negative or 0. If PARNAM is to be a time-varying parameter, the keyword "INSTANCES" and a value for NUMINST must be entered.

4a. [INSTNAM]

4b. [Mltarr Zonarr IZ]

   After each Item 3 for which the keyword "INSTANCES" is not entered, read Item 4b and not Item 4a.

   After each Item 3 for which the keyword "INSTANCES" is entered, read Item 4a and Item 4b for each instance. NCLU repetitions of Item 4b are required. Each repetition of Item 4b

is called a parameter cluster. The NCLU repetitions of Item 4b follow each repetition of Item 4a when PARNAM is time varying.

FOR EACH STRESS PERIOD

Read item 5a only if NRCHOP = 2

5a. INRECH INIRCH [OPTIONS2]

Read item 5b only if NRCHOP is not 2.

5b. INRECH [OPTIONS2]

If UNSTRUCTURED option is used, then read items 6a and 6b.

6a. [RECH(INIRCH)] -- U1DREL if NPRCH=0 and if INRECH ≥ 0

Note that INIRCH is equal to the number of nodes in the top layer if NRCHOP =1 or 3.

6b. [Pname [Iname] [IRCHPF]] -- if NPRCH > 0 and if INRECH > 0

Either Item 6a or Item 6b may be read, but not both. Item 6b, if read, is repeated INRECH times. Iname is read if Pname is a time-varying parameter.

Otherwise, if UNSTRUCTURED option is not used, then read items 7a anf 7b for structured input.

7a. [RECH(NCOL,NROW)] -- U2DREL if NPRCH=0 and if INRECH ≥ 0

7b. [Pname [Iname] [IRCHPF]] -- if NPRCH > 0 and if INRECH > 0

Either Item 7a or Item 7b may be read, but not both. Item 7b, if read, is repeated INRECH times. Iname is read if Pname is a time-varying parameter.

If UNSTRUCTURED option is used, then read item 8a

8a. [IRCH(INIRCH)] -- U1DINT If NRCHOP=2 and if INIRCH > = 0

Otherwise, if UNSTRUCTURED option is not used, then read item 8b for structured input

8b. [IRCH(NCOL,NROW)] -- U2DINT If NRCHOP=2 and if INIRCH > = 0

Item 9 is read only if the flag on option2 “INCONC” is supplied. Item 11 is read as many times as the flag IRCHCONC(ICOMP) > 0. Item 11 is the array of concentrations for each of the non-zero concentration components.

Read item 9 only if OPTIONS2 is used with keyword INRCHZONES [nzones] where nzones is the number of zones for which a recharge time-series is implemented.

If UNSTRUCTURED option is used, then read item 9a

9a. [IZNRCH(INIRCH)] -- U1DREL

Otherwise, if UNSTRUCTURED option is not used, then read item 9b for structured input

9b. [IZNRCH(NCOL,NROW)] -- U2DREL

Read item 10 only if OPTIONS2 is used with keyword INSELEV [iflag] where iflag greater than zero.

If UNSTRUCTURED option is used, then read item 10a

10a. [SELEV(INIRCH)] -- U1DREL

Otherwise, if UNSTRUCTURED option is not used, then read item 10b for structured input

10b. [SELEV(NCOL,NROW)] -- U2DREL

Read item 11 only if OPTIONS2 is used with keyword INCONC is used. Item 11 is read MCOMPT times (as many times as there are mobile solute components plus one if temperature simulation is also conducted, as long as the flag IRCHCONC is greater than zero for that component).

If UNSTRUCTURED option is used, then read item 11a

11a. [RCHCONC(INIRCH)] -- U1DREL

Otherwise, if UNSTRUCTURED option is not used, then read item 11b for structured input

11b. [RCHCONC(NCOL,NROW)] -- U2DREL

Explanation of Variables Read by the RCH Package

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPRCH—is the number of recharge parameters.

NRCHOP—is the recharge option code. Recharge fluxes are defined in a layer variable, RECH, with one value for each vertical column. Accordingly, recharge is applied to one cell in each vertical column, and the option code determines which cell in the column is selected for recharge.

1—Recharge is only to the top grid layer.

2—Vertical distribution of recharge is specified in layer variable IRCH.

3—Recharge is applied to the highest active cell in each vertical column. A constant-head node intercepts recharge and prevents deeper infiltration. Note that if the top-most layer is inactive for unstructured grids, this option assigns all recharge flux to the first active node in the layers below. Hence, if there is a vertical nesting involved, with multiple active nodes underlying an inactive node, then the recharge is not spread over all of these underlying active underlying nodes. The quantity of water, however, is conserved for the prescribed recharge rate.

IRCHCB—is a flag and a unit number.

If IRCHCB > 0, cell-by-cell flow terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control.

If IRCHCB ≤ 0, cell-by-cell flow terms will not be written.

OPTIONS1 are keywords that activates options:

SEEPELEV indicates that the recharge is limited when the water level reaches that elevation. Recharge can reduce to zero and below (indicating discharge) indicating the development of a seepage face.

RTS [mxrtzones] indicates that the recharge time-series input is also provided and the number following the keyword RTS is the maximum number of zones for which the transient recharge time-series is provided.

CONCENTRATION (or CONC) indicates that species concentrations will also be input for transport simulations. If this option is not present, the concentration of all species in recharge water is assumed to be zero.

MXNDRCH—is the maximum number of nodes to which recharge is applied in a simulation. This parameter is read only when the UNSTRUCTURED option is used with NRCHOP=2 (whereby the nodes to which recharge is applied are a user input).

IRCHCONC—is a flag indicating if concentration of a component is to be read or not.

If IRCHCONC =0, then do not read concentration array for this species and it will be taken as zero.

If IRCHCONC =1, then read concentration array for this species.

PARNAM—is the name of a parameter to be defined. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter to be defined. For the RCH Package, the only allowed parameter type is RCH, which defines values of the recharge flux.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NCLU—is the number of clusters required to define a non-time-varying parameter or one instance of a time varying parameter. Each repetition of Item 4b is a cluster (variables Mltarr, Zonarr, and IZ). Usually only one cluster is used to define a RCH non-time-varying parameter or an instance of a time-varying parameter; however, more than one cluster is acceptable.

INSTANCES—is an optional keyword that designates a parameter as time varying. The keyword is not case sensitive; that is, any combination of the same characters with different case can be used. If ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, PARNAM is non-time-varying and NUMINST should not be present.

NUMINST—is the number of instances for a time-varying parameter, where each instance is a list of river reaches and associated properties. If the keyword ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, NUMINST should not be present.

INSTNAM—is the name of an instance associated with the parameter named in the corresponding Item 3. The instance name can be 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent. Instance names must be unique for a parameter, but instance names may be reused for different parameters.

MItarr—is the name of the multiplier array to be used to define cell values that are determined by a parameter. The name "NONE" means that there is no multiplier array, and the cell values will be set equal to Parval.

Zonarr—is the name of the zone array to be used to define the cells that are associated with a parameter. The name "ALL" means that there is no zone array, and all cells in the layer are associated with the parameter.

IZ—is up to 10 zone numbers (separated by spaces) that define the cells that are associated with a parameter. These values are not used if Zonarr is specified as "ALL." Values can be positive or negative, but 0 is not allowed. The end of the line, a zero value, or a non-numeric entry terminates the list of values.

INRECH—is the RECH read flag. Its function depends on whether or not parameters are being used.

If no parameters are being used (NPRCH = 0):

If INRECH ≥ 0, a layer variable of recharge fluxes, RECH, is read.

If INRECH < 0, recharge rates from the preceding stress period are used.

If parameters are being used (NPRCH > 0):

If INRECH > 0, INRECH is the number of parameters that will be used to define RECH in the current stress period. Items 6b (for unstructured grids) or 7b (for structured grids) define the names of the parameters.

If INRECH < 0, recharge parameters from the preceding stress period are used.

INRECH = 0 is not allowed. That is, when parameters are used, at least one parameter must be specified each stress period.

INIRCH—is the IRCH read flag, which is read only if NRCHOP is two:

If INIRCH ≥ 0, a layer variable of layer numbers (IRCH) is read for a structured grid. For an unstructured grid, INIRCH is further equal to the number of nodes for which recharge values are read in the simulation, with the nodes being identified in array IRCH.

If INIRCH < 0, the variable (IRCH) used in the preceding stress period is reused.

OPTIONS2 are keywords that activate options:

INSELEV [iflag] indicates that a seepage elevation is input for this stress period. This condition is maintained till another INSELEV keyword changes it at a later stress period. This flag has to be on for at least the first stress period if SEEPELEV option was selected under OPTIONS1 on the first data line. Otherwise, the seepage elevations will not be read in Item 10 a or 10 b. The flag takes on integer values which indicate the following.

If INSELEV > 0, then an array of seepage elevations is read to limit recharge such that water levels do not rise above the seepage elevation surface.

If INSELEV = 0 then recharge is not constrained for this stress period and henceforth till another INSELEV flag changes it.

If INSELEV < 0, the seepage elevations of the preceding stress period is reused.

INRCHZONES [iflag] indicates that the zones for input of recharge time-series are input for this stress period. This condition is maintained till another INRCHZONES keyword

changes it at a later stress period. The flag (INIZNRCH) takes on integer values which indicate the following.

If INIZNRCH > 0, then an array of zonal indices is read for providing time-series recharge values to those zones. The value of INIZNRCH is equal to the maximum number of zones of recharge for the model.

If INIZNRCH = 0 then zonal indices for recharge time-series input is not read for this stress period and henceforth till another INSELEV flag changes it.

If INIZNRCH < 0, the zonal distribution of the preceding stress period is reused.

INCONC indicates that concentrations will be input for species with non-zero concentrations in recharge water for transport simulations. If this option is not provided, concentrations of components in recharge water will not be read for this stress period and will be assumed to be the same as for the previous stress period.

RECH—is the recharge flux (LT^{-1}). Read only if INRECH is greater than or equal to zero and if NPRCH = 0.

Pname—is the name of a parameter that will be used to define the RECH variable in the current stress period. Read INRECH values if NPRCH > 0 and INRECH > 0.

Iname—is an instance name that is read only if Pname is a time-varying parameter. Multiple instances of the same parameter are not allowed in a stress period.

IRCHPF—is an optional format code for printing the RECH variable after it has been defined by parameters. The format codes are the same as those used in the U2DREL array reading utility subroutine.

IRCH—is the layer number that defines the layer in each vertical column where recharge is applied when a structured MODFLOW grid is used. For an unstructured grid, IRCH is the node number to which the recharge is applied, where the list includes INIRCH number of nodes. Read only if NRCHOP is two and if INIRCH is greater than or equal to zero.

IZNRCH—is the array of zonal indices for applying a recharge time series to zones in the model. This recharge input is independent of the stress period input and total recharge is the sum of recharge via stress periods and the time series.

SELEV—is the seepage elevation allowed. Recharge is constrained to limit water levels from rising above the seepage elevation.

TRANSIENT RECHARGE FILE

If recharge is provided to the model via a tabular time-series file independent of the stress periods (i.e., flag INIZNRCH 0), then this file is also opened in the NAME file under the keyword RTS. The time-series file is in free format and includes one data entry per row. Data on each row is as follows:

Each Row: **TMSTRT TMEND TMFACTR RCHZ(1) RCHZ(2) … RCHZ(INIZNRCH)**

TMSTRT—is the starting time for a recharge event.

TMEND—is the ending time for a recharge event.

TMFACTR—is a multiplying factor applied to all recharge zones for the current recharge event.

RCHZ(1), RCHZ(2), … RCHZ(INIZNRCH)—are the recharge rates for each zone for a recharge event.

Note that the recharge values for all zones between times TMSTRT and TMEND are added to the recharge array input in the RCH file. Also, if there is a gap between the TMEND of one record, and the TMSTRT of the next, then zero recharge is added to the model from the time-series input for that time period.

EVAPOTRANSPIRATION (EVT) PACKAGE INPUT INSTRUCTIONS

Input to the Evapotranspiration (EVT) Package is read from the file that is type “EVT” in the Name File. All single-valued variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format.

Note that the EVT package has been extended from the MODFLOW-2005 version to also include time varying PET conditions that are prescribed irrespective of stress periods. Thus, PET fluxes can be applied at a smaller temporal scale than stress periods, in a manner similar to time varying heads or fluxes of the Flow and Head Boundary (FHB) package. The time varying PET flux conditions are implemented by supplying zonal identification in the EVT input file, with temporally varying PET fluxes supplied as a time series for each zone, via a separate file. ***Note that if PET is supplied as a time series, then PET values supplied for stress periods in the EVT file (still required as input) are ignored***.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. [PARAMETER NPEVT]

This optional item must start with the word "PARAMETER".

The third entry in item 2a below (IETFACTOR) is required only if transport simulation is active (ITRNSP ≠ 0)

2a. NEVTOP IEVTCB IETFACTOR [OPTIONS1]

Item 2b is read only if IUNSTR = 1 and NEVTOP = 2

2b. MXNDEVT

Item 2c is read only if IETFACTOR = 1 and transport simulation is active (ITRNSP ≠ 0)

2c. ETFACTOR(MCOMP)

The factors are input in free format if the option "FREE" is specified in the Basic Package input file; otherwise, the variables all have 10-character fields.

3. [PARNAM PARTYP Parval NCLU [INSTANCES NUMINST]]

Repeat Item 3 combined with the indicated repetitions of Item 4 NPEVT times. Items 3 and 4 are not read if NPEVT is negative or 0.

If PARNAM is to be a time-varying parameter, the keyword "INSTANCES" and a value for NUMINST must be entered.

4a. [INSTNAM]

4b. [MItarr Zonarr IZ]

After each Item 3 for which the keyword "INSTANCES" is not entered, read Item 4b and not Item 4a.

After each Item 3 for which the keyword "INSTANCES" is entered, read Item 4a and Item 4b for each instance.

NCLU repetitions of Item 4b are required. Each repetition of Item 4 is called a parameter cluster. The NCLU repetitions of Item 4b follow each repetition of Item 4a when PARNAM is time varying.

FOR EACH STRESS PERIOD

Read item 5a only if NEVTOP = 2

5a. **INSURF INEVTR INEXDP INIEVT [OPTIONS2]**

Read item 5b only if NEVTOP is not 2.

5b. **INSURF INEVTR INEXDP INIZNEVT [OPTIONS2]**

If UNSTRUCTURED option is used then read items 6 THROUGH 10.

6. **[SURF(INIEVT)]** -- U2DREL If INSURF ≥ 0

7. **[EVTR(INIEVT)]** -- U2DREL If NPEVT = 0 and if INEVTR ≥ 0

8. **[Pname [Iname] [IEVTPF]] -- if NPEVT > 0 and if INEVTR > 0**

   Either Item 7 or Item 8 may be read, but not both. Item 8, if read, is repeated INEVTR times. Iname is read if Pname is a time-varying parameter.

9. **[EXDP(INIEVT)] -- U2DREL If INEXDP ≥ 0**

10. **[IEVT(INIEVT)] -- U2DINT If NEVTOP = 2 and if INIEVT ≥ 0**

Note in items 6 through 10 that that INIEVT is equal to the number of nodes in the top layer if INIEVT = 1 or 3. Items 6 through 10 are read for unstructured input only.

Read Item 11 only if the flag on option INEVTZONES, [inznevt] > 0

11. **[IZNEVT(INIEVT)]** -- U2DINT

Otherwise, if UNSTRUCTURED option is not used then read items 11 through 15 for structured input.

12. **[SURF(NCOL,NROW)] -- U2DREL If INSURF ≥ 0**

13. **[EVTR(NCOL,NROW)] -- U2DREL If NPEVT = 0 and if INEVTR ≥ 0**

14. **[Pname [Iname] [IEVTPF]] -- if NPEVT > 0 and if INEVTR > 0**

    Either Item 14 or Item 15 may be read, but not both. Item 14, if read, is repeated INEVTR times. Iname is read if Pname is a time-varying parameter.

15. **[EXDP(NCOL,NROW)] -- U2DREL If INEXDP ≥ 0**

16. **[IEVT(NCOL,NROW)] -- U2DINT If NEVTOP = 2 and if INIEVT ≥ 0**

Read item 17 only if optional keyword **INEVTZONES** is read and the flag **[iniznevt] > 0**

17. **[IZNEVT(NCOL,NROW)]** -- U2DINT

Explanation of Variables Read by the EVT Package

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPEVT—is the number of evapotranspiration parameters.

NEVTOP—is the evapotranspiration (ET) option code. ET variables (ET surface, maximum ET rate, and extinction depth) are specified in layer variables, SURF, EVTR, and EXDP, with one value for each vertical column. Accordingly, ET is calculated for one cell in each vertical column. The option codes determine the cell within a column for which ET will be calculated.

1—ET is calculated only for cells in the top grid layer.

2—The cell for each vertical column is specified by the user in variable IEVT.

3—ET is applied to the highest active cell in each vertical column. A constant-head node supplies the required ET and prevents ET from the domain. Note that if the top-most layer is inactive for unstructured grids, this option assigns all ET flux to the first active node in the layers below. Hence if there is a vertical nesting involved, with multiple active nodes underlying an inactive node then the ET is not spread over all of these underlying active underlying nodes. The quantity of water however, is conserved for the prescribed maximum ET rate.

IEVTCB—is a flag and a unit number.

If IEVTCB > 0, cell-by-cell flow terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control.

If IEVTCB ≤ 0, cell-by-cell flow terms will not be written.

OPTIONS1 are keywords that activate options:

ETS [mxetzones] indicates that the potential evapotranspiration (PET) time-series input is also provided and the number following the keyword ETS, [**mxetzones].** is the maximum number of zones for which the PET time-series is provided.

IETFACTOR—is a flag indicating if ET removes contaminant mass with water or not.

If IETFACTOR > 0, contaminant mass can be removed with evapotranspiration and the factor ETFACTOR is read for each component in data item 2c. ETFACTOR determines the fraction of mass of the component that leaves with water. Thus, if ET removes water but leaves behind the solutes, the ETRACTOR is zero. At the other extreme, if all solutes leave with water then the ET factor is set to 1.

If IETFACTOR = 0, ET leaves behind contaminant mass and only water is removed from the modeled system. The ETFACTOR is automatically set to zero and is not read.

If IETFACTOR < 0, contaminant mass is fully removed with evapotranspiration. The ETFACTOR is automatically set to 1 and is not read.

MXNDEVT—is the maximum number of nodes on which ET is applied in a simulation. This parameter is read only when IUNSTR=1 (for a unstructured grid) with NEVTOP=2 (whereby the nodes on which ET is applied are a user input).

ETFACTOR(MCOMP)—is the fraction of mass of the component that leaves with water.

If ETFACTOR = 0 then water exits the domain via the ET boundary but all component mass is left behind.

If ETFACTOR = 1 then mass of component leaves with water as is the case in other outflow boundary conditions.

If ETFACTOR ≥ 0 or ≤ 1 then only the prescribed fraction of component mass leaves the domain with water at the ET boundary.

PARNAM—is the name of a parameter to be defined. This name can consist of 1 to 10 characters and is not case sensitive; that is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter to be defined. For the EVT Package, the only allowed parameter type is EVT, which defines values of the maximum ET flux, variable EVTR.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NCLU—is the number of clusters required to define a non-time-varying parameter or one instance of a time-varying parameter. Each repetition of Item 4b is a cluster (variables Mltarr, Zonarr, and IZ). Usually only one cluster is used to define an EVT non-time-varying parameter or an instance of a time-varying parameter; however, more than one cluster is acceptable.

INSTANCES—is an optional keyword that designates a parameter as time varying. The keyword is not case sensitive; that is, any combination of the same characters with different case can be used. If ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, PARNAM is non-time-varying and NUMINST should not be present.

NUMINST—is the number of instances for a time-varying parameter, where each instance is a list of river reaches and associated properties. If the keyword ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, NUMINST should not be present.

INSTNAM—is the name of an instance associated with the parameter named in the corresponding Item 3. The instance name can be 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent. Instance names must be unique for a parameter, but instance names may be reused for different parameters.

MItarr—is the name of the multiplier array to be used to define the values that are determined by a parameter. The name "NONE" means that there is no multiplier array, and the values will be set equal to Parval.

Zonarr—is the name of the zone array to be used to define the cells that are associated with a parameter. The name "ALL" means that there is no zone array, and all cells are associated with the parameter.

IZ—is up to 10 zone numbers (separated by spaces) that define the cells that are associated with a parameter. These values are not used if Zonarr is specified as "ALL." Values can be positive or negative, but 0 is not allowed. The end of the line, a zero value, or a non-numeric entry terminates the list of values.

INSURF—is the ET surface (SURF) read flag.

If **INSURF≥ 0**, a layer variable containing the ET surface elevation (SURF) will be read.

If **INSURF < 0**, the ET surface from the preceding stress period will be reused.

INEVTR—is the EVTR read flag. Its function depends on whether or not parameters are being used.

If no parameters are being used (NPEVT=0):

If **INEVTR ≥ 0**, a layer variable containing the maximum ET rate (EVTR) will be read.

If **INEVTR < 0**, the maximum ET rate from the preceding stress period will be reused.

If parameters are being used (NPEVT>0):

If **INEVTR > 0**, INEVTR is the number of parameters that will be used to define EVTR in the current stress period. Item 8 defines the names of the parameters.

If **INEVTR < 0**, EVT parameters from the preceding stress period are used.

INEVTR = 0 is not allowed. That is, when parameters are used, at least one parameter must be specified each stress period

INEXDP—is the extinction depth (EXDP) read flag.

If **INEXDP ≥ 0**, a layer variable containing the extinction depth (EXDP) will be read.

If **INEXDP < 0**, the extinction depth from the preceding stress period will be reused.

INIEVT—is the layer indicator (IEVT) read flag that is read only if the ET option (NEVTOP) is equal to two.

If **INIEVT ≥ 0**, an array containing the layer indicators (IEVT) will be read for a structured grid. For an unstructured grid, INIEVT is further equal to the number of nodes for which ET values are read in the simulation, with the nodes being identified in the array IEVT. For an unstructured grid, INIEVT is further equal to the number of nodes for which ET values are read in the simulation, with the nodes being identified in the array IEVT.

If **INIEVT < 0**, layer indicators used during the preceding stress period will be reused.

OPTIONS2 are keywords that activate options:

INEVTZONES [iniznevt] indicates that the zones for input of PET time-series are input for this stress period. The flag **[iniznevt]** takes on integer values which indicate the following.

If **[iniznevt]** > 0, then an array of zonal indices is read for providing time-series PET values to those zones. The value of **[iniznevt]** is equal to the maximum number of zones of PET for the model. Note that the zones can be redistributed at every stress period by having a positive value of [iniznevt].

If **[iniznevt]** < 0, the zonal distribution of the preceding stress period is reused.

SURF—is the elevation of the ET surface. This variable is read only if INSURF ≥ 0

EVTR—is the maximum ET flux [volumetric flow rate per unit area (LT-1)]. This variable is read only if INEVTR ≥ 0 and if NPEVT=0. Contrary to the usual convention in MODFLOW, EVTR values should be specified as positive values even though they represent an outflow from the groundwater system.

Pname—is the name of a parameter that will be used to define the EVTR variable in the current stress period. Read INEVTR values if NPEVT > 0 and INEVTR > 0.

Iname—is an instance name that is read only if Pname is a time-varying parameter. Multiple instances of the same parameter are not allowed in a stress period.

IEVTPF—is an optional format code for printing the EVTR variable after it has been defined by parameters. The format codes are the same as those used in the U2DREL array reading utility subroutine.

EXDP—is the ET extinction depth. This variable is read only if INEXDP ≥ 0.

IEVT—is the layer indicator variable. For each horizontal location, IEVT indicates the layer from which ET is removed, when a structured MODFLOW grid is used (IUNSTR=0). For an unstructured grid input (IUNSTR=1), IEVT is the node number on which the ET is applied, where the list includes INIEVT number of nodes. Read only if NEVTOP is two and if INIEVT is greater than or equal to zero.

IZNEVT—is the array of zonal indices for applying a PET time series to zones in the model. This PET input is independent of the stress period input, which is ignored when the zonal time series are provided.

TRANSIENT PET TIME-SERIES FILE

If the PET flux is provided to the model via a time-series file independent of the stress periods (i.e., flag INIZNEVT 0), then this file is also opened in the NAME file under the keyword EVS. The time-series file is in free format and includes one data entry per row. Data on each row is as follows:

Each Row: **TMSTRT TMEND TMFACTR EVTZ(1) EVTZ(2) … EVTZ(INIZNRCH)**

TMSTRT—is the starting time for a PET input.

TMEND—is the ending time for a PET input.

TMFACTR—is a multiplying factor applied to all PET zones for the current time period.

EVTZ (1), EVTZ (2), … EVTZ (INIZNEVT)—are the PET rates for each zone for the current time period.

Note that if there is a gap between the TMEND of one record, and the TMSTRT of the next, then zero PET is applied to the model for that time period.

SEGMENTED EVAPOTRANSPIRATION (ETS) PACKAGE INPUT INSTRUCTIONS

Input to the Segmented Evapotranspiration (ETS) Package is read from the file that is type "ETS" in the Name File. All single-valued variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format. The time series input extension done for RCH and EVT packages is not yet incorporated into the ETS package.

FOR EACH SIMULATION

0. [#Text]

   Item 0 is optional—“#” must be in column 1. Item 0 can be repeated multiple times.

1. [***PARAMETER*** NPETS]

   This optional item must start with the word “PARAMETER”.

2a. NETSOP IETSCB NPETS NETSEG IESFACTOR

Item 2b is read only for an unstructured grid and NETSOP = 2

2b. MXNDETS

Item 2C is read only if transport is active and IESFACTOR=1

2b. ESFACTOR(MCOMP)

3. [PARNAM PARTYP Parval NCLU [INSTANCES NUMINST]]

   Repeat Item 3 combined with the indicated repetitions of Item 4 NPETS times. Items 3 and 4 are not read if NPETS is negative or 0.

   If PARNAM is to be a time-varying parameter, the keyword “INSTANCES” and a value for NUMINST must be entered.

4a. [INSTNAM]

4b. [Mltarr Zonarr IZ]

   After each Item 3 for which the keyword “INSTANCES” is not entered, read Item 4b and not Item 4a.

   After each Item 3 for which the keyword “INSTANCES” is entered, read Item 4a and Item 4b for each instance.

   NCLU repetitions of Item 4b are required. Each repetition of Item 4 is called a parameter cluster. The NCLU repetitions of Item 4b follow each repetition of Item 4a when PARNAM is time varying.

FOR EACH STRESS PERIOD

Read item 5a if NETSOP = 2 or if NETSEG > 1.

5a. INETSS INETSR INETSX [INIETS [INSGDF]]

Read item 5b if NETSOP is not equal to 2 and NETSEG =1

5b. INETSS INETSR INETSX [INSGDF]

If UNSTRUCTURED option is used, then read items 6 through 12.

6. [ETSS(INIETS)] -- U2DREL If INETSS ≥ 0

7. [ETSR(INIETS)] -- U2DREL If NPETS = 0 and if INETSR ≥ 0

8. [Pname [Iname] [IETSPF]] -- if NPETS > 0 and if INETSR > 0

Either Item 7 or Item 8 may be read, but not both. Item 8, if read, is repeated INETSR times. Iname is read if Pname is a time-varying parameter.

9. [ETSX(INIETS)] -- U2DREL If INETSX ≥ 0

10. [IETS(INIETS)] -- U2DINT If NETSOP = 2 and if INIETS ≥ 0

Read items 11 and 12 below only if NETSEG > 1. (i.e., there are more than one segment to the ET function), and INSGDF ≥ 0

11. [PXDP(INIETS)] -- U2DREL If NETSET > 1 and INSGDF ≥ 0

12. [PETM(INIETS)] -- U2DINT If NETSET > 1 and INSGDF ≥ 0

Note in items 6 through 12 that INIETS is equal to the number of nodes in the top layer if NETSOP = 1 or 3. Items 6 through 12 are read for unstructured input only.

If NETSEG > 1, (NETSEG − 1) repetitions of items 11 and 12 are read. If NETSEG > 2, items 11 and 12 are read for the uppermost segment intersection, followed by repetitions of items 11 and 12 for successively lower intersections.

Otherwise, if UNSTRUCTURED option is not used, then read items 13 through 19 for structured input

13. [ETSS(NCOL,NROW)] -- U2DREL If INETSS ≥ 0

14. [ETSR(NCOL,NROW)] -- U2DREL If NPETS = 0 and if INETSR ≥ 0

15. [Pname [Iname] [IETSPF]] -- if NPETS > 0 and if INETSR > 0

Either Item 15 or Item 16 may be read, but not both. Item 13, if read, is repeated INETSR times. Iname is read if Pname is a time-varying parameter.

16. [ETSX(NCOL,NROW)] -- U2DREL If INETSX ≥ 0

17. [IETS(NCOL,NROW)] -- U2DINT If NETSOP = 2 and if INIETS ≥ 0

Read items 11 and 12 below only if NETSEG > 1. (i.e., there are more than one segment to the ET function), and INSGDF ≥ 0

18. [PXDP(NCOL,NROW)] -- U2DREL If NETSET > 1 and INSGDF ≥ 0

19. [PETM(NCOL,NROW)] -- U2DINT If NETSET > 1 and INSGDF ≥ 0

If NETSEG > 1, (NETSEG − 1) repetitions of items 18 and 19 are read. If NETSEG > 2, items 18 and 19 are read for the uppermost segment intersection, followed by repetitions of items 18 and 19 for successively lower intersections.

Explanation of Variables Read by the ETS Package

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPETS—is the number of evapotranspiration parameters.

NETSOP—is the evapotranspiration (ET) option code. ET variables (ET surface, maximum ET rate, and extinction depth) are specified in layer variables, SURF, ETSR, and EXDP, with one value for each vertical column. Accordingly, ET is calculated for one cell in each vertical column. The option codes determine the cell within a column for which ET will be calculated.

1—ET is calculated only for cells in the top grid layer.

2—The cell for each vertical column is specified by the user in variable IETS.

3—ET is applied to the highest active cell in each vertical column. A constant-head node supplies the required ET and prevents ET from occurring from the domain. Note that if the top-most layer is inactive for unstructured grids, this option assigns all ET flux to the first active node in the layers below. Hence if there is a vertical nesting involved, with multiple active nodes underlying an inactive node then the ET is not spread over all of these active underlying nodes. The quantity of water however, is conserved for the prescribed ET rate if the cell can provide the ET rate without becoming dry.

IETSCB—is a flag and a unit number.

If IETSCB > 0, cell-by-cell flow terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control.

If IETSCB ≤ 0, cell-by-cell flow terms will not be written.

NETSEG—is the number of segments used to define the relation of evapotranspiration rate to hydraulic head in the interval where the evapotranspiration rate is variable.

IESFACTOR—is flag indicating that a solute removal fraction with ET will be read when transport is active.

If IESFACTOR =1, solute removal fraction with ET flux is read in ESFACTOR array for each component simulated.

If IESFACTOR = 0, All solutes are left behind when ET removes water and the ESFACTOR array is not read.

MXNDETS—is the maximum number of nodes on which ET is applied in a simulation. This parameter is read only for an unstructured grid with NETSOP=2 (whereby the nodes on which ET is applied are a user input).

ESFACTOR(MCOMP)—is the array for input of fraction of solute (for all 1 to MCOMP solutes) that is extracted with ET. A value of zero means all solutes are left behind with ET flux only extracting the water. A value of one indicates that solutes leave in an advective manner with the flux of water as it would be extracted by a well. A fraction allows for partial extraction of solutes with the evapotranspiration flux, to allow for partial volatility of solute.

PARNAM—is the name of a parameter to be defined. This name can consist of 1 to 10 characters and is not case sensitive; that is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter to be defined. For the ETS Package, the only allowed parameter type is ETS, which defines values of the maximum ET flux, variable ETSR.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NCLU—is the number of clusters required to define a non-time-varying parameter or one instance of a time-varying parameter. Each repetition of Item 4b is a cluster (variables Mltarr, Zonarr, and IZ). Usually only one cluster is used to define an ETS non-time-varying parameter or an instance of a time-varying parameter; however, more than one cluster is acceptable.

INSTANCES—is an optional keyword that designates a parameter as time varying. The keyword is not case sensitive; that is, any combination of the same characters with different case can be used. If ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, PARNAM is non-time-varying and NUMINST should not be present.

NUMINST—is the number of instances for a time-varying parameter, where each instance is a list of river reaches and associated properties. If the keyword ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, NUMINST should not be present.

INSTNAM—is the name of an instance associated with the parameter named in the corresponding Item 3. The instance name can be 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent. Instance names must be unique for a parameter, but instance names may be reused for different parameters.

MItarr—is the name of the multiplier array to be used to define the values that are determined by a parameter. The name "NONE" means that there is no multiplier array, and the values will be set equal to Parval.

Zonarr—is the name of the zone array to be used to define the cells that are associated with a parameter. The name "ALL" means that there is no zone array, and all cells are associated with the parameter.

IZ—is up to 10 zone numbers (separated by spaces) that define the cells that are associated with a parameter. These values are not used if Zonarr is specified as "ALL." Values can be positive or negative, but 0 is not allowed. The end of the line, a zero value, or a non-numeric entry terminates the list of values.

INETSS—is the ET surface (ETSS) read flag.

If INETSS≥ 0, a layer variable containing the ET surface elevation (ETSS) will be read.

If INETSS < 0, the ET surface from the preceding stress period will be reused.

INETSR—is the ETSR read flag. Its function depends on whether or not parameters are being used.

If no parameters are being used (NPETS=0):

If INETSR ≥ 0, a layer variable containing the maximum ET rate (ETSR) will be read.

If INETSR < 0, the maximum ET rate from the preceding stress period will be reused.

If parameters are being used (NPETS>0):

If INETSR > 0, INETSR is the number of parameters that will be used to define ETSR in the current stress period. Item 15 defines the names of the parameters.

If INETSR < 0, ETS parameters from the preceding stress period are used.

INETSR = 0 is not allowed. That is, when parameters are used, at least one parameter must be specified each stress period

INETSX—is the extinction depth (ETSX) read flag.

If INETSX ≥ 0, a layer variable containing the extinction depth (ETSX) will be read.

If INETSX < 0, the extinction depth from the preceding stress period will be reused.

INIETS—is the layer indicator (IETS) read flag. It is read if the ET option (NETSOP) is equal to two or if NETSEG > 1. If NETSEG = 1 and NETSOP is not equal to two, INIETS is ignored and IETS is not read.

If INIETS ≥ 0, an array containing the layer indicators (IETS) will be read for a structured grid. For an unstructured grid, INIETS is further equal to the number of nodes for which ET values are read in the simulation, with the nodes being identified in the array IETS.

If INIETS < 0, layer indicators used during the preceding stress period will be reused.

INSGDF—is the segment definition read flag. It is read only if NETSEG > 1.

If INSGDF ≥ 0, two layer variables to define PXDP and PETM for each of (NETSEG – 1) segment intersections are read from items 10 and 11, respectively, of the ETS1 input file.

If INSGDF < 0, PXDP and PETM from the preceding stress period will be reused.

ETSS—is the elevation of the ET surface. This variable is read only if INETSS ≥ 0

ETSR—is the maximum ET flux [volumetric flow rate per unit area (LT^{-1})]. This variable is read only if INETSR ≥ 0 and if NPETS=0. Contrary to the usual convention in MODFLOW, ETSR values should be specified as positive values even though they represent an outflow from the groundwater system.

Pname—is the name of a parameter that will be used to define the ETSR variable in the current stress period. Read INETSR values if NPETS > 0 and INETSR > 0.

Iname—is an instance name that is read only if Pname is a time-varying parameter. Multiple instances of the same parameter are not allowed in a stress period.

IETSPF—is an optional format code for printing the ETSR variable after it has been defined by parameters. The format codes are the same as those used in the U2DREL array reading utility subroutine.

ETSX—is the ET extinction depth. This variable is read only if INETSX ≥ 0.

IETS—is the layer indicator variable. For each horizontal location, IETS indicates the layer from which ET is removed when a structured MODFLOW grid is used. For an unstructured grid, IETS is the node number to which the ET is applied, where the list includes INIETS number of nodes. Read only if NETSOP is two and if INIETS is greater than or equal to zero.

PXDP—is a proportion of the extinction depth (dimensionless), measured downward from the ET surface, which, with PETM, defines the shape of the relation between the evapotranspiration rate and head. The value of PXDP must be between 0.0 and 1.0, inclusive. Repetitions of PXDP and PETM are read in sequence such that the first occurrence represents the bottom of the first segment, and subsequent repetitions represent the bottom of successively lower segments. Accordingly, PXDP values for later repetitions (representing lower segments) should be greater than PXDP values for earlier repetitions.

PETM—is a proportion of the maximum evapotranspiration rate (dimensionless) which, with PXDP, defines the shape of the relation between the evapotranspiration rate and head. The value of PETM should be between 0.0 and 1.0, inclusive. Repetitions of PXDP and PETM are read in sequence such that the first occurrence represents the bottom of the first segment, and subsequent repetitions represent the bottoms of successively lower

segments. Accordingly, PETM values for later repetitions (representing lower segments) generally would be less than PETM values for earlier repetitions.

WELL (WEL) PACKAGE INPUT INSTRUCTIONS

Input to the Well (WEL) Package is read from the file that has type "WEL" in the Name File. Optional variables are shown in brackets. All variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format. Extra considerations are provided in the WEL package than those of MODFLOW-2005. First, an option is provided via keyword AUTOFLOWREDUCE, whereby a simulated well will adjust pumping (extraction only) according to supply under bottom-hole conditions. Reduced well pumping is then output to a file IUNITAFR if that option is also set. Also, if the WELLBOT option is set, then input for the well bottom-hole elevation is also required for every entry. This input is to be provided before input of any auxiliary variable. The well bottom can be any value above the bottom of the cell (GWF or CLN) and can also be above the top of the cell. If water levels fall to or below this level, the well does not pump.

Also, if CLN cells exist in a simulation with a structured grid, the input requirements for these wells may be different and the user can input CLN cell number instead of layer, row and column (or the cell number). Therefore, an option is provided to separately read the CLN cell numbers and their pumping rates. This option of separate CLN input may also be used with unstructured grids; however, the global node numbers and their pumping rates may also be directly read. The global matrix contains the GWF cells first, followed by the CLN domain cells and the global node numbers are ordered accordingly. Also, for the case of CLN cells within a structured finite-difference grid, parameter wells are only applied to the GWF cells and not to the CLN cells.

For transport simulations, the concentrations of species components are included for wells using the auxiliary variables AUX $C0_1$, AUX $C0_2$, etc. Input for the auxiliary variables follows input for cell location and the pumping rate.

FOR EACH SIMULATION

0. [#Text]

   Item 0 is optional—“#” must be in column 1. Item 0 can be repeated multiple times.

1a. [***PARAMETER*** NPWEL MXL]

This optional item must start with the word “PARAMETER”.

2. MXACTW IWELCB [Option]

3. [PARNAM PARTYP Parval NLST [***INSTANCES*** NUMINST]]

   Repeat Item 3 combined with the indicated repetitions of Item 4 NPWEL times. Items 3 and 4 are not read if NPWEL is negative or 0.

   If PARNAM is to be a time-varying parameter, the keyword “INSTANCES” and a value for NUMINST must be entered.

4a. [INSTNAM]

4b. Layer Row Column Qfact [wbot] [xyz]

   Enter Item 4b if a structured grid is used

4c. Node Qfact [wbot] [xyz]

   Enter Item 4c if an unstructured grid is used

   After each Item 3 for which the keyword “INSTANCES” is not entered, read Item 4b, or 4c and not Item 4a.

   After each Item 3 for which the keyword “INSTANCES” is entered, read Item 4a and Item 4b, or 4c for each instance.

   NLST repetitions of Item 4b or 4c are required; they are read by subroutine ULSTRD. (SFAC of the ULSTRD utility subroutine applies to Qfact). The NLST repetitions of Item 4b or 4c follow each repetition of Item 4a when PARNAM is time varying.

FOR EACH STRESS PERIOD

5. ITMP NP ITMPCLN

6a. Layer Row Column Q [wbot] [xyz]

   Omit Item 6a if unstructured grid is used

(ITMP repetitions of Item 6a are read by subroutine ULSTRD if ITMP > 0. (SFAC of the ULSTRD utility subroutine applies to Q.) Item 6a is not read if ITMP is negative or zero.

6b. Node Q [wbot] [xyz]

Omit Item 6b if structured grid is used

(ITMP repetitions of Item 6b are read by subroutine ULSTRD if ITMP > 0. (SFAC of the ULSTRD utility

subroutine applies to Q.) Item 6b is not read if ITMP is negative or zero.

6c. ICLNNODE Q [wbot] [xyz]

Omit Item 6c if ITMPCLN = 0.

(ITMPCLN repetitions of Item 6c are read by subroutine ULSTRD if ITMPCLN > 0. (SFAC of the ULSTRD utility subroutine applies to Q.) Item 6c is not read if ITMPCLN is negative or zero.

7. [Pname [Iname]]

(Item 7 is repeated NP times. It is not read if NP is negative or 0. Iname is read if Pname is a time-varying parameter.)

Explanation of Variables Read by the WEL Package

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPWEL—is the number of well parameters.

MXL—is the maximum number of wells that will be defined using parameters.

MXACTW—is the maximum number of wells in use during any stress period, including those that are defined using parameters.

IWELCB—is a flag and a unit number.

If IWELCB > 0, cell-by-cell flow terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control.

If IWELCB = 0, cell-by-cell flow terms will not be written.

If IWELCB < 0, well recharge for each well will be written to the listing file when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control.

Option—is an optional list of character values.

"AUXILIARY abc" or "AUX abc"—defines an auxiliary variable, named "abc", which will be read for each well as part of Items 4 and 6. Up to 20 variables can be specified, each of which must be preceded by "AUXILIARY" or "AUX." These variables will not be used by the Ground-Water Flow Process, but they will be available for use by other processes. The auxiliary variable values will be read after the Q variable. Note that for transport, the auxiliary variable for concentration is *AUX C##* where *C##* is the solute species number (for example, *C01* indicates solute species 1; *C20* indicates solute species 20).

"NOPRINT"—specifies that lists of wells will not be written to the Listing File.

"AUTOFLOWREDUCE" —specifies that the well pumping rate is reduced as per the flux to the well node under bottom-hole conditions. If well pumping is in a subsurface node, the bottom elevation of the cell is used to evaluate the bottom-hole elevation. If well pumping is in a CLN cell, the bottom elevation of the CLN cell is used to evaluate the bottom-hole elevation. Thus, in essence, the pumping reverts to constant head conditions with reduced flux if water levels try to fall below the bottom-hole elevation. The full pumping flux is resumed if the water levels bounce back as a result of changing stress conditions in the system. If this option is not specified, then the well pumping rate is maintained as per the MODFLOW-2005 well boundary condition.

"IUNITAFR" —specifies that wells with pumping rates that have been automatically reduced will be written to an output file. The unit number for this output file must immediately follow the "IUNITAFR" keyword option. If this option is used then a file of type "DATA" should be included in the Name file with a unit number that matches the unit number specified here. This option can also be used to specify the unit number for the listing file, in which case, the reduced flow information will be written to the listing file.

"WELLBOT" —specifies that the bottom-hole elevations of the wells are input after input of pumping rate for each well in the simulation. This input is provided for every stress period.

PARNAM—is the name of a parameter. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter. For the WEL Package, the only allowed parameter type is Q, which defines values of the volumetric recharge rate.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NLST—is the number of wells in a non-time-varying parameter. For a time-varying parameter, NLST is the number of wells in each instance.

INSTANCES—is an optional keyword that designates a parameter as time varying. The keyword is not case sensitive; that is, any combination of the same characters with different case can be used. If ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, PARNAM is non-time-varying and NUMINST should not be present.

NUMINST—is the number of instances for a time-varying parameter, where each instance is a list of river reaches and associated properties. If the keyword ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, NUMINST should not be present.

INSTNAM—is the name of an instance associated with the parameter named in the corresponding Item 3. The instance name can be 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent. Instance names must be unique for a parameter, but instance names may be reused for different parameters.

Layer—is the layer number of the model cell that contains the well.

Row—is the row number of the model cell that contains the well.

Column—is the column number of the model cell that contains the well.

ICLNNODE—is the Connected Linear Network-node number that contains the well.

Node—is the global node number of the model cell (GWF cell or CLN cell) that contains the well. The global node number of a GWF cell for a structured grid may be computed as (KLAY-1)*NROW*NCOL + (IROW-1)*NCOL + JCOL where KLAY is the layer number, IROW is the row number and JCOL is the column number of the GWF Process cell. For a CLN cell, the global node number is the CLN cell node number plus the total number of GWF Process cells.

Qfact—is the factor used to calculate well recharge rate from the parameter value. The recharge rate is the product of Qfact and the parameter value.

[wbot]—specifies that bottom-hole elevation of the well if the WELLBOT option is used.

[xyz]—represents the values of the auxiliary variables for a well that have been defined in Item 2. The values of auxiliary variables must be present in each repetition of Items 4 and 6 if they are defined in Item 2. The values must be specified in the order used to define the variables in Item 2.

ITMP—is a flag and a counter for subsurface nodes.

If ITMP < 0, non-parameter well data from the last stress period for subsurface nodes will be reused.

ITMP ≥ 0, ITMP will be the number of non-parameter wells read for the current stress period for subsurface nodes.

NP—is the number of parameters in use in the current stress period.

ITMPCLN—is a flag and a counter. Note that ITMPCLN is read only if the CLN domain exists in a simulation. This is required for a structured grid in which layer, row and column assignments are read for each node, to accommodate input of pumping conditions within conduit- geometry CLN cells. For unstructured grids, well input for CLN cells may be provided here, or may be directly provided via the ITMP well nodes using their global node numbers.

If ITMPCLN < 0, non-parameter well data from the last stress period for CLN cells will be reused.

If ITMPCLN ≥ 0, ITMPCLN will be the number of non-parameter wells read for the current stress period for CLN cells.

Q—is the volumetric recharge rate. A positive value indicates recharge and a negative value indicates discharge (pumping).

Pname—is the name of a parameter that is being used in the current stress period. NP parameter names will be read.

Iname—is an instance name that is read only if Pname is a time-varying parameter. Multiple instances of the same parameter are not allowed in a stress period.

DRAIN (DRN) PACKAGE INPUT INSTRUCTIONS

Input to the Drain (DRN) Package is read from the file that has type "DRN" in the Name File. Optional variables are shown in brackets. All variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—“#” must be in column 1. Item 0 can be repeated multiple times.

1. [PARAMETER NPDRN MXL]

This optional item must start with the word “PARAMETER”.

2. MXACTD IDRNCB [Option]

3. [PARNAM PARTYP Parval NLST [INSTANCES NUMINST]]

Repeat Item 3 combined with the indicated repetitions of Item 4 NPDRB times. Items 3 and 4 are not read if NPDRN is negative or 0.

If PARNAM is to be a time-varying parameter, the keyword “INSTANCES” and a value for NUMINST must be entered.

4a. [INSTNAM]

4b. [Layer Row Column Elevation Condfact [xyz]]

Omit Item 4b if an unstructured grid is used

4c. Node Condfact [xyz]

Omit Item 4c if a structured grid is used

After each Item 3 for which the keyword “INSTANCES” is not entered, read Item 4b or 4c and not Item 4a.

After each Item 3 for which the keyword “INSTANCES” is entered, read Item 4a and Item 4b or 4c for each instance.

NLST repetitions of Item 4b or 4c are required; they are read by subroutine ULSTRD. (SFAC of the ULSTRD utility subroutine applies to Condfact). The NLST repetitions of Item 4b or 4c follow each repetition of Item 4a when PARNAM is time varying.

FOR EACH STRESS PERIOD

5. ITMP NP

6a. Layer Row Column Elevation Cond [xyz]

Omit Item 6a if an unstructured grid is used

6b. Node Elevation Cond [xyz]

Omit Item 6b if a structured grid is used

ITMP repetitions of Item 6a or 6b are read by subroutine ULSTRD if ITMP > 0. (SFAC of the ULSTRD utility subroutine applies to Cond.) Item 6a or 6b is not read if ITMP is negative or 0.

7. [Pname [Iname]]

(Item 7 is repeated NP times. Item 7 is not read if NP is negative or 0. Iname is read if Pname is a time-varying parameter.)

Explanation of Variables Read by the DRN Package:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPDRN—is the number of drain parameters.

MXL—is the maximum number of drain cells that will be defined using parameters.

MXACTD—is the maximum number of drain cells in use during any stress period, including those that are defined using parameters.

IDRNCB—is a flag and a unit number.

If IDRNCB > 0, cell-by-cell flow terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control.

If IDRNCB = 0, cell-by-cell flow terms will not be written.

If IDRNCB < 0, drain leakage for each drain cell will be written to the listing file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control.

Option—is an optional list of character values.

"AUXILIARY abc" or "AUX abc"—defines an auxiliary variable, named "abc", which will be read for each drain as part of Items 4 and 6. Up to 20 variables can be specified, each of which must be preceded by "AUXILIARY" or "AUX." These variables will not be used by the Ground-Water Flow Process, but they will be available for use by other processes. The auxiliary variable values will be read after the Cond variable.

"NOPRINT"—specifies that lists of drains will not be written to the Listing File.

PARNAM—is the name of a parameter. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter. For the DRN Package, the only allowed parameter type is DRN, which defines values of the drain hydraulic conductance.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NLST—is the number of drain in a non-time-varying parameter. For a time-varying parameter, NLST is the number of drain cells in each instance.

INSTANCES—is an optional keyword that designates a parameter as time varying. The keyword is not case sensitive; that is, any combination of the same characters with different case can be used. If INSTANCES is present, it must be followed by a value for NUMINST. If INSTANCES is absent, PARNAM is non-time-varying and NUMINST should not be present.

NUMINST—is the number of instances for a time-varying parameter, where each instance is a list of river reaches and associated properties. If the keyword INSTANCES is present, it must be followed by a value for NUMINST. If INSTANCES is absent, NUMINST should not be present.

INSTNAM—is the name of an instance associated with the parameter named in the corresponding Item 3. The instance name can be 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent. Instance names must be unique for a parameter, but instance names may be reused for different parameters.

Layer—is the layer number of the cell containing the drain.

Row—is the row number of the cell containing the drain.

Column—is the column number of the cell containing the drain.

Node—is the node number of the model cell that contains the drain.

Elevation—is the elevation of the drain.

Condfact—is the factor used to calculate drain hydraulic conductance from the parameter value. The conductance is the product of Condfact and the parameter value.

[xyz]—represents the values of the auxiliary variables for a drain that have been defined in Item 2. The values of auxiliary variables must be present in each repetition of Items 4 and 6 if they are defined in Item 2. The values must be specified in the order used to define the variables in Item 2.

ITMP—is a flag and a counter.

If ITMP < 0, non-parameter drain data from the last stress period will be reused.

If ITMP ≥ 0, ITMP will be the number of non-parameter drains read for the current stress period.

NP—is the number of parameters in use in the current stress period.

Cond—is the hydraulic conductance of the interface between the aquifer and the drain.

Pname—is the name of a parameter that is being used in the current stress period. NP parameter names will be read.

Iname—is an instance name that is read only if Pname is a time-varying parameter. Multiple instances of the same parameter are not allowed in a stress period.

GENERAL-HEAD BOUNDARY (GHB) PACKAGE INPUT INSTRUCTIONS

Input to the General-Head Boundary (GHB) Package is read from the file that has file type "GHB" in the Name File. Optional variables are shown in brackets. All variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—“#” must be in column 1. Item 0 can be repeated multiple times.

1. [PARAMETER NPGHB MXL]

This optional item must start with the word “PARAMETER”.

2. MXACTB IGHBCB [Option]

3. [PARNAM PARTYP Parval NLST [INSTANCES NUMINST]]

Repeat Item 3 combined with the indicated repetitions of Item 4 NPGHB times. Items 3 and 4 are not read if NPGHB is negative or 0.

If PARNAM is to be a time-varying parameter, the keyword “INSTANCES” and a value for NUMINST must be entered.

4a. [INSTNAM]

4b. [Layer Row Column Bhead Condfact [xyz]]

Omit Item 4b if an unstructured grid is used

4c. Node Bhead Condfact [xyz]

Omit Item 4c if a structured grid is used

After each Item 3 for which the keyword “INSTANCES” is not entered, read Item 4b or 4c and not Item 4a.

After each Item 3 for which the keyword “INSTANCES” is entered, read Item 4a and Item 4b or 4c for each instance.

NLST repetitions of Item 4b or 4c are required; they are read by subroutine ULSTRD. (SFAC of the ULSTRD utility subroutine applies to Condfact). The NLST repetitions of Item 4b or 4c follow each repetition of Item 4a when PARNAM is time varying.

FOR EACH STRESS PERIOD

5. ITMP NP

6a. Layer Row Column Bhead Cond [xyz]

Omit Item 6a if an unstructured grid is used

6b. Node Bhead Cond [xyz]

Omit Item 6b if a structured grid is used

ITMP repetitions of Item 6a or 6b are read by subroutine ULSTRD if ITMP > 0. (SFAC of the ULSTRD utility subroutine applies to Cond.) Item 6a or 6b are not read if ITMP is negative or 0.

7. [Pname [Iname]]

(Item 7 is repeated NP times. Item 7 is not read if NP is negative or 0. Iname is read if Pname is a time-varying parameter.)

Explanation of Variables Read by the GHB Package:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPGHB—is the number of general-head boundary parameters.

MXL—is the maximum number of general-head-boundary cells that will be defined using parameters.

MXACTB—is the maximum number of general-head boundary cells in use during any stress period, including those that are defined using parameters.

IGHBCB—is a flag and a unit number.

If IGHBCB > 0, cell-by-cell flow terms will be written to the unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control.

If IGHBCB = 0, cell-by-cell flow terms will not be written.

If IGHBCB < 0, boundary leakage for each GHB cell will be written to the listing file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control.

Option—is an optional list of character values.

"AUXILIARY abc" or "AUX abc"—defines an auxiliary variable, named "abc", which will be read for each general-head boundary as part of Items 4 and 6. Up to 20 variables can be specified, each of which must be preceded by "AUXILIARY" or "AUX." These variables will

not be used by the Ground-Water Flow Process, but they will be available for use by other processes. The auxiliary variable values will be read after the Cond variable.

"NOPRINT"—specifies that lists of general-head boundary cells will not be written to the Listing File.

PARNAM—is the name of a parameter. This name can consist of 1 to 10 characters and is not case sensitive; that is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter to be defined. For the GHB Package, the only allowed parameter type is GHB, which defines values of the general-head boundary hydraulic conductance.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NLST—is the number of head-dependent boundaries in a non-time-varying parameter. For a time-varying parameter, NLST is the number of head-dependent boundaries in each instance.

INSTANCES—is an optional keyword that designates a parameter as time varying. The keyword is not case sensitive; that is, any combination of the same characters with different case can be used. If INSTANCES is present, it must be followed by a value for NUMINST. If INSTANCES is absent, PARNAM is non-time-varying and NUMINST should not be present.

NUMINST—is the number of instances for a time-varying parameter, where each instance is a list of river reaches and associated properties. If the keyword INSTANCES is present, it must be followed by a value for NUMINST. If INSTANCES is absent, NUMINST should not be present.

INSTNAM—is the name of an instance associated with the parameter named in the corresponding Item 3. The instance name can be 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent. Instance names must be unique for a parameter, but instance names may be reused for different parameters.

Layer—is the layer number of the cell affected by the head-dependent boundary.

Row—is the row number of the cell affected by the head-dependent boundary.

Column—is the column number of the cell affected by the head-dependent boundary.

Node—is the node number of the model cell affected by the head-dependent boundary.

Bhead—is the boundary head.

Condfact—is the factor used to calculate hydraulic conductance from the parameter value. The conductance is the product of Condfact and the parameter value.

[xyz]—represents the values of the auxiliary variables for a boundary that have been defined in Item 2. The values of auxiliary variables must be present in each repetition of Items 4 and 6 if they are defined in Item 2. The values must be specified in the order used to define the variables in Item 2.

ITMP—is a flag and a counter.

If ITMP < 0, non-parameter GHB data from the preceding stress period will be reused.

If ITMP ≥ 0, ITMP is the number of non-parameter general-head boundaries read for the current stress period.

NP—is the number of parameters in use in the current stress period.

Cond—is the hydraulic conductance of the interface between the aquifer cell and the boundary.

Pname—is the name of a parameter that is being used in the current stress period. NP parameter names will be read.

Iname—is an instance name that is read only if Pname is a time-varying parameter. Multiple instances of the same parameter are not allowed in a stress period.

DRAIN WITH RETURN FLOW (DRT) AND GHB-Q PACKAGE INPUT INSTRUCTIONS

Input to the DRT1 Package is read from the file that has type “DRT” in the name file. Optional variables are shown in brackets. All variables are free format if the option “FREE” is specified in

the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format.

Note that the DRT package is also used to provide a GHB-Q condition. This condition applies a GHB instead of a drain, with return flow occurring just as in the DRT application. A negative drain conductance value indicates that a GHB condition should be applied instead of a drain condition, and the drain elevation is interpreted as the GHB head elevation.

When this package is used with transport, the solute can be manipulated before return flow occurs. Solute mass or concentration can be added or removed as per treatment that may be provided to the water before returning it.

FOR EACH SIMULATION

0. [#Text]

   Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. MXADRT IDRTCB NPDRT MXL [Option]

2. [PARNAM PARTYP Parval NLST]

Item 3a is read only for a structured grid

3a. Layer Row Column Elevation Condfact [LayR RowR ColR Rfprop] [IDCHNGTYP] [xyz]

Item 3b is read only for an unstructured grid

3b. Node Elevation Condfact [NodeR Rfprop] [IDCHNGTYP] [xyz]

   NLST repetitions of Item 3 records are required; they are read by module ULSTRD (Harbaugh and others, 2000). (SFAC of the ULSTRD utility module applies to Condfact.)

   Repeat Items 2 and 3 for each parameter to be defined (that is, NPDRT times). **Items 2 and 3 are omitted if NPDRT = 0.**

FOR EACH STRESS PERIOD

4. ITMP NP

Item 5a is read only for a structured grid

5a. Layer Row Column Elevation Cond [LayR RowR ColR Rfprop] [IDCHNGTYP] [xyz]

Item 5b is read only for an unstructured grid

5b. Node Elevation Cond [NodeR Rfprop] [IDCHNGTYP] [xyz]

ITMP repetitions of Item 5 records are read by module ULSTRD (Harbaugh and others, 2000) if ITMP > 0. (SFAC of the ULSTRD utility module applies to Cond). Item 5 is not read if ITMP≤□0.

6. Pname

(Item 6 is repeated NP times. It is not read if NP ≤□0.)

Explanation of Variables Read by the DRT Package:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

MXADRT—is the maximum number of drain-return cells in use during any stress period, including those defined using parameters. **Recipient cells are not included in MXADRT**.

IDRTCB—is a flag and a unit number.

If IDRTCB > 0, it is the unit number to which DRT1-Package cell-by-cell flow terms will be written when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control (Harbaugh and others, 2000). IDRTCB must be a unit number associated with a file listed with type "DATA (BINARY)" or "DATAGLO(BINARY)" in the name file.

If IDRTCB = 0, DRT1-Package cell-by-cell flow terms will not be written.

If IDRTCB < 0, drain leakage for each drain-return cell and return flow to each recipient cell will be written to the LIST file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control.

NPDRT—is the number of drain-return parameters.

MXL—is the maximum number of drain-return cells that will be defined using parameters. Recipient cells are not included in MXL. Option—is an optional list of character values.

Option—is an optional list of character values

"AUXILIARY abc" or "AUX abc"—defines an auxiliary variable (Harbaugh and McDonald, 1996a, p. 9, item 4), named "abc," which will be read for each drain as part of items 3 and 5. Up to five variables can be specified, each of which must be preceded by "AUXILIARY" or "AUX." These variables will not be used by the Ground-Water Flow Process, but they will be available for use by other processes. The auxiliary variable values will be read after the Cond variable.

"CBCALLOCATE" or "CBC"—indicates that memory should be allocated to store cell-by-cell flow for each drain in order to make these flows available for use in other packages.

"NOPRINT"—indicates that the list of drain-return cells will not be printed.

"RETURNFLOW"—activates the return-flow option of the DRT1 Package. If "RETURNFLOW" is listed as an option, LayR, and, optionally, RowR, ColR, and Rfprop are read from items 3 and (or) 5.

"CHANGEC"—indicates that the concentration of solutes or temperature (for thermal component of a simulation) may be changed before returning the water to the return-flow location.

PARNAM—is the name of a parameter to be defined. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter to be defined. For the DRT1 Package, the only allowed parameter type is "DRT," which defines values of the drain hydraulic conductance.

Parval—is the parameter value. This parameter value may be overridden by a value in the Sensitivity Process input file or by a value generated by the Parameter-Estimation Process.

NLST—is the number of drain-return cells included in the parameter.

Node—is the layer number of the cell containing the drain.

Layer—is the layer number of the cell containing the drain.

Row—is the row number of the cell containing the drain.

Column—is the column number of the cell containing the drain.

Elevation—is the elevation of the drain. If the next entry (Condfact) is negative, then the DRT boundary acts as a GHB-Q condition and this variable is the elevation of the water level for the GHB condition.

Condfact—is the factor used to calculate drain hydraulic conductance from the parameter value. The conductance (L^2/T) is the product of Condfact and the parameter value. If the **Condfact** is negative, then the DRT boundary acts as a GHB-Q condition and **Condfact** is the GHB hydraulic conductance for the GHB condition.

NodR—is a flag and, if greater than 0, a node number. If auxiliary variables are being read, NodR must be greater than zero, so that Rfprop is read. NodR is not read if "RETURNFLOW" is not listed as an option in item 1.

If NodR > 0, it is the node number of the recipient cell.

If NodR = 0, there is no return flow for the drain cell, and Rfprop are not read.

LayR—is a flag and, if greater than 0, a layer number. If auxiliary variables are being read, LayR must be greater than zero, so that RowR, ColR, and Rfprop are read. LayR is not read if "RETURNFLOW" is not listed as an option in item 1.

If LayR > 0, it is the layer number of the recipient cell.

If LayR = 0, there is no return flow for the drain cell, and RowR, ColR, and Rfprop are not read.

RowR—is the row number of the recipient cell. RowR is not read if "RETURNFLOW" is not listed as an option in item 1.

ColR—is the column number of the recipient cell. ColR is not read if "RETURNFLOW" is not listed as an option in item 1.

Rfprop—is the return-flow proportion. Valid values are in the range 0.0 to 1.0, inclusive. Rfprop is the proportion of the drain flow, if any, calculated for the drain-return cell simulated as returning to the recipient cell. If Rfprop equals 0.0, the return-flow capability is deactivated for the cell. Rfprop is not read if "RETURNFLOW" is not listed as an option in item 1. If **Condfact** above is negative, then the DRT boundary acts as a GHB-Q condition and this variable **Rfprop** is the flux rate applied to the return flow node (instead of a proportion of the extracted flux).

[IDCHNGTYP] —is an index depicting the type of change that is made to the return-flow solutes or heat, for transport simulations. This index facilitates a change of the return flow concentration or solute mass as per some treatment. The index is read only if CHANGEC option is invoked for the simulation

If **IDCHNGTYP = 0**, there is no change and the drained concentration (or temperature) is reapplied at the return-flow location.

If **IDCHNGTYP = 1**, a fixed concentration (or temperature) amount is added to the drained concentration (or temperature) before reapplying the water at the return-flow location. The concentration or temperature amounts are provided as AUXILIARY variables (C01, C02, etc. for concentrations, or TMPR for heat). The values are positive if solute concentration (or temperature) are added to the drained amount and negative if solute concentration (or temperature) are to be subtracted from the drained value.

If **IDCHNGTYP = 2**, a fixed mass (or heat amount) is added to the drained solute mass (or heat) before reapplying the water at the return-flow location. The mass or heat amounts are provided as AUXILIARY variables (C01, C02, etc. for concentrations, or TMPR for heat). The values are positive if solute mass (or heat) are added to the drained amount and negative if solute mass (or heat) are to be subtracted from the drained value. Note that for heat, the equation is divided by $\rho_w c_w$ therefore the additional heat input should also be divided by the same amount (please see the section on het transport for details).

If **IDCHNGTYP = 3,** the concentration is set to a fixed concentration (or temperature) value before reapplying the water at the return-flow location. The concentration or temperature values are provided as AUXILIARY variables (C01, C02, etc. for concentrations, or TMPR

for heat). Note that solute (or heat) may be added or subtracted to the water to bring it to that concentration (or temperature) value.

If **IDCHNGTYP = 4**, the mass is set to a fixed mass (or heat) value before reapplying the water at the return-flow location. The mass (or heat) values are provided as AUXILIARY variables (C01, C02, etc. for solute mass, or TMPR for heat). Note that solute (or heat) may be added or subtracted to the water to bring it to that mass (or heat) value.

If **IDCHNGTYP = 5**, the concentration is **reduced** to a fixed concentration (or temperature) value before reapplying the water at the return-flow location, if the extracted concentration is above the prescribed value, otherwise the extracted value is applied. The prescribed concentration or temperature values are provided as AUXILIARY variables (C01, C02, etc. for concentrations, or TMPR for heat). Note that solute (or heat) will be subtracted from the water to bring it to that concentration (or temperature) value. This change type is typical of a reverse osmosis process that removes solutes up to a given value.

[xyz]—is up to five auxiliary variables for a drain-return cell that have been defined in item 1. The auxiliary variables must be present in each repetition of items 3 and 5 record if they are defined in item 1.

ITMP—is a flag and a counter.

If ITMP < 0, non-parameter drain-return data from the last stress period will be reused.

If ITMP ≥0, ITMP will be the number of non-parameter drain-return cells read for the current stress period.

NP—is the number of drain-return parameters in use in the current stress period.

Cond—is the hydraulic conductance of the interface between the aquifer and the drain.

Pname—is the name of a parameter being used in the current stress period. NP parameter names will be read.

SINK WITH RETURN FLOW (QRT) PACKAGE INPUT INSTRUCTIONS

Input to the QRT1 Package is read from the file that is attached to type “QRT” in the name file. Optional variables are shown in brackets. All variables are free format if the option “FREE” is

specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format. **Note that the extracted Q value is positive in the QRT dataset as it relates strictly to extraction of water and reapplying of the extracted water, while the opposite may not be realistic.** Also note that the QRT input can be optionally continuous, as in the FHB Package instead of varying with stress periods, using the TRANSIENTQ optional keyword.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. MXAQRT MXRTCELLS IQRTCB NPQRT MXL [Option]

2. [PARNAM PARTYP Parval NLST]

Item 3a is read only for a structured grid

3a. Layer Row Column SinkQfact NumRT [Rfprop] [IQCHNGTYP] [xyz]

Item 3b is read only for an unstructured grid

3b. Node RTNum SinkQfact NumRT [Rfprop] [IQCHNGTYP] [xyz]

NLST repetitions of Item 3 records are required; they are read by module ULSTRD (Harbaugh and others, 2000). (SFAC of the ULSTRD utility module applies to SinkQ.)

Repeat Items 2 and 3 for each parameter to be defined (that is, NPQRT times). ***Items 2 and 3 are omitted if NPQRT = 0.***

Input Items T1 through T2 below are read only if option TRANSIENTQ is set. This option reads the hydrographs for the sink cells instead of using the stress periods to vary the rates.

Items T1 provide the time values for interpolation of extraction rates when TRANSIENTQ is set. Include NBDQTIM times in data item T1b.

T1a. Data: IQRTUN CNSTM

T1b. Data: BDQTIM(NBDQTIM)

Items T2 provide the sink extraction rate values for interpolation of extraction rates when TRANSIENTQ is set. Include NBDQTIM times in data item T2b.

T2a. Data: IQRTUN CNSTM

T2b. Data: Node BDQV(NBDQTIM)

FOR EACH STRESS PERIOD

4. ITMP NP

Item 5a is read only for a structured grid

5a. Layer Row Column SinkQ NumRT [Rfprop] [IQCHNGTYP] [xyz]

Item 5b is read only for an unstructured grid

5b. Node SinkQ NumRT [Rfprop] [IQCHNGTYP] [xyz]

ITMP repetitions of Item 5 records are read by module ULSTRD (Harbaugh and others, 2000) if ITMP > 0. (SFAC of the ULSTRD utility module applies to SinkQ). Item 5 is not read if ITMP≤□0.

6. NodQRT(NumRT,IsinkQ) (U1DINT)

ITMP repetitions of Item 6 records are read by module U1DINT if ITMP > 0, once for each of the IsinkQ extraction points or sinks simulated. The array contains the NumRT return flow cells associated with sink IsinkQ. Item 6 is not read if ITMP≤□0

7. Pname

(Item 7 is repeated NP times. It is not read if NP ≤□0.)

Explanation of Variables Read by the QRT Package:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

MXAQRT—is the maximum number of "Sink-return" sink cells in use during any stress period, including those defined using parameters. **Recipient cells are not included in MXAQRT**.

MXRTCELLS—is the maximum number of recipient cells that may exist in the simulation during any stress period. MXRTCELLS is used to dimension the array of recipient cells for all sinks and should be larger than or equal to the number of recipient cells that may be listed in the simulation during any stress period.

IQRTCB—is a flag and a unit number.

If IQRTCB > 0, it is the unit number to which QRT1-Package cell-by-cell flow terms will be written when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control (Harbaugh and others, 2000). IQRTCB must be a unit number associated with a file listed with type "DATA(BINARY)" or "DATAGLO(BINARY)" in the name file.

If IQRTCB = 0, QRT1-Package cell-by-cell flow terms will not be written.

If IQRTCB < 0, Sink leakage for each Sink-return cell and return flow to each recipient cell will be written to the LIST file when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in Output Control.

NPQRT—is the number of Sink-return parameters.

MXL—is the maximum number of "Sink-return" sink cells that will be defined using parameters. Recipient cells are not included in MXL. Option—is an optional list of character values.

Option—is an optional list of character values

"**AUXILIARY abc" or "AUX abc**"—defines an auxiliary variable (Harbaugh and McDonald, 1996a, p. 9, item 4), named "abc," which will be read for each Sink as part of items 3 and 5. Up to five variables can be specified, each of which must be preceded by "AUXILIARY" or "AUX." These variables will not be used by the Ground-Water Flow Process, but they will be available for use by other processes. The auxiliary variable values will be read after the Cond variable.

"**CBCALLOCATE**" or "**CBC**"—indicates that memory should be allocated to store cell-by-cell flow for each Sink in order to make these flows available for use in other packages.

"**RETURNFLOW**"—activates the return-flow option of the QRT1 Package. If "RETURNFLOW" is listed as an option, NumRT, and optionally, Rfprop are read from items 3 and (or) 5.

"**CHANGEC**"—indicates that the concentration of solutes or temperature (for thermal component of a simulation) or the mass of solutes in returned water may be altered before returning the water to the return-flow location(s).

"**TRANSIENTQ nbdqtim**"— the keyword TRANSZIENTQ indicates that FHB style hydrograph input will be provided for every sink and the interpolated value will be used instead of the value provided in the stress period list for the sink rate. The keyword is followed by an integer value NBDQTIM which indicates the number of interpolation points on the hydrograph. If the value of NBDQTIM is negative, then it indicates that a step function will be used instead of interpolating between the data points.

"**AUTOFLOWREDUCE**" —specifies that the well pumping rate is reduced as per the flux to the well node under bottom-hole conditions. If well pumping is in a subsurface node, the bottom elevation of the cell is used to evaluate the bottom-hole elevation. If well pumping is in a CLN cell, the bottom elevation of the CLN cell is used to evaluate the bottom-hole elevation. Thus, in essence, the pumping reverts to constant head conditions with reduced flux if water levels try to fall below the bottom-hole elevation. The full pumping flux is resumed if the water levels bounce back as a result of changing stress conditions in the system. If this option is not specified, then the well pumping rate is maintained as per the MODFLOW-2005 well boundary condition.

"**IUNIT_AFR_QRT iu_afr_qrt**" —specifies that extraction rates that have been automatically reduced will be written to an output file. The unit number for this output file, iu_afr_qrt, must immediately follow the "IUNIT_AFR_QRT" keyword option. If this option is used, then a file of type "DATA" should be included in the Name file with a unit number that matches the unit number specified here for iu_afr_qrt. This option can also be used to specify the unit number for the listing file, in which case, the reduced flow information will be written to the listing file.

PARNAM—is the name of a parameter to be defined. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter to be defined. For the QRT1 Package, the only allowed parameter type is "SinkQ," which defines values of the volumetric flux rate for the sink.

Parval—is the parameter value. This parameter value may be overridden by a value in the Sensitivity Process input file or by a value generated by the Parameter-Estimation Process.

NLST—is the number of Sink-return cells included in the parameter.

Node—is the layer number of the cell containing the Sink.

Layer—is the layer number of the cell containing the Sink.

Row—is the row number of the cell containing the Sink.

Column—is the column number of the cell containing the Sink.

SinkQfact—is the factor used to calculate the volumetric flux rate of the Sink from the parameter value. The volumetric flux rate of the Sink is the product of SinkQfact and the parameter value.

NumRT—is a flag and, if greater than 0, a layer number. If auxiliary variables are being read, NumRT must be greater than zero, so that Rfprop is read. NumRT is not read if "RETURNFLOW" is not listed as an option in item 1.

If NumRT > 0, it is the number of recipient cells.

If NumRT = 0, there is no return flow for the Sink cell, and Rfprop are not read.

Rfprop—is the return-flow proportion. Valid values are in the range 0.0 to 1.0, inclusive. Rfprop is the proportion of the Sink flow, if any, that is returned to the recipient cells. If Rfprop equals 0.0, the return-flow capability is deactivated for the cell. Rfprop is not read if "RETURNFLOW" is not listed as an option in item 1.

[IQCHNGTYP] —is an index depicting the type of change that is made to the return-flow of solutes or heat, for transport simulations. This index facilitates a change of the return flow concentration or solute mass as per some treatment. The index is read only if CHANGEC option is invoked for the simulation.

If **IQCHNGTYP = 0**, there is no change and the extracted concentration (or temperature) is reapplied at the return-flow location.

If **IQCHNGTYP = 1**, a fixed concentration (or temperature) amount is added to the extracted concentration (or temperature) before reapplying the water at the return-flow location. The concentration or temperature amounts are provided as AUXILIARY variables (C01, C02, etc. for concentrations, or TMPR for heat). The values are positive if solute concentration (or temperature) are added to the extracted amount and negative if solute concentration (or temperature) are to be subtracted from the extracted value.

If **IQCHNGTYP = 2**, a fixed mass (or heat amount) is added to the extracted solute mass (or heat) before reapplying the water at the return-flow location. The mass or heat amounts are provided as AUXILIARY variables (C01, C02, etc. for concentrations, or TMPR for heat). The values are positive if solute mass (or heat) are added to the extracted amount and negative if solute mass (or heat) are to be subtracted from the extracted value. Note that for heat, the equation is divided by $\rho_w c_w$ therefore the additional heat input should also be divided by the same amount (please see the section on het transport for details).

If **IQCHNGTYP = 3**, the concentration is set to a fixed concentration (or temperature) value before reapplying the water at the return-flow location. The concentration or temperature values are provided as AUXILIARY variables (C01, C02, etc. for concentrations, or TMPR for heat). Note that solute (or heat) may be added or subtracted to the water to bring it to that concentration (or temperature) value.

If **IQCHNGTYP = 4**, the mass is set to a fixed mass (or heat) value before reapplying the water at the return-flow location. The mass (or heat) values are provided as AUXILIARY variables (C01, C02, etc. for solute mass, or TMPR for heat). Note that solute (or heat) may be added or subtracted to the water to bring it to that mass (or heat) value.

If **IQCHNGTYP = 5**, the concentration is **reduced** to a fixed concentration (or temperature) value before reapplying the water at the return-flow location, if the extracted concentration

is above the prescribed value, otherwise the extracted value is applied. The prescribed concentration or temperature values are provided as AUXILIARY variables (C01, C02, etc. for concentrations, or TMPR for heat). Note that solute (or heat) will be subtracted from the water to bring it to that concentration (or temperature) value. This change type is typical of a reverse osmosis process that removes solutes up to a given value.

[xyz]—is up to five auxiliary variables for a Sink-return cell that have been defined in item 1. The auxiliary variables must be present in each repetition of items 3 and 5 record if they are defined in item 1.

NBDQTIM—is the number of interpolation points on the hydrograph of Q vs. time. A negative value is entered for NBDQTIM if a stepped representation of the hydrograph is simulated between the data points instead of interpolation. Thus, the value will be held constant till the next time value in the table is reached. For example, if there are 3 time-values in a table of time versus flux, and the time values are 0.0, 365.0, 1000.0, and if the flux values are 100, 500, 200, then the flux value of 100 is applied from 0 to 365 days, the flux value of 500 is applied from 365 to 1000 days, and a flux value of 200 is applied beyond 1000 days of the simulation

Note that if adaptive time stepping is used with a stepped representation of the sink flow rate changes through time, then the time step value will adjust to exactly hit the data points such that the flux is exactly integrated.

IQRTUN—is the unit number on which data lists will be read. The same or different unit numbers can be used to read lists in data items T1 listing the time values and T2 listing the sink flow rates.

CNSTM—is a constant multiplier for data list BDQTIM (data item T1b) and BDFV (data item T2b).

BDQTIM—is simulation time at which values of the sink flow rate will be read. NBDQTIM values are required.

IQRTN—is the node number of the sink cell for which transient flow rates are specified.

BDQV—is the volumetric rate of flow at the QRT sink cells. A list of NBDQTIM values must be specified for all the MXAQRT cells in the domain.

ITMP—is a flag and a counter.

If ITMP < 0, non-parameter Sink-return data from the last stress period will be reused.

If ITMP ≥ 0, ITMP will be the number of non-parameter Sink-return cells read for the current stress period.

NP—is the number of Sink-return parameters in use in the current stress period.

SinkQ—is the volumetric flux (L^3/T) from the Sink.

NodQRT(NumRT,IsinkQ) —is the node number of the NumRT return flow nodes associated with sink IsinkQ.

Pname—is the name of a parameter being used in the current stress period. NP parameter names will be read.

Arrays for QRT module:

QRTF(1,ii) = Node number (or Layer Number for structured grid)

QRTF(2,ii) = (Row Number for structured grid)

QRTF(3,ii) = (Column Number for structured grid)

QRTF(4,ii) = Extraction stress (SinkQ)

QRTF(5,ii) = Number of nodes on which return occurs (NumRT)

QRTF(6,ii) = Return fraction (Rfprop)

QRTF(6,ii) = Actual extraction (may be less than SinkQ due to autoflowreduce)

NodQRT(NumRT, IsinkQ) – Keep a cumulative list in a 1-D array of maximum length MXRTCELLS.

QRTFLOW(NumRT, IsinkQ) – Also kept in a cumulative list in a 1-D array.

BDQTIM(NBDQTIM) – Time values for input of a table of time versus sink fluxes.

BDQV(NBDQTIM, MXAQRT) – Sink flux values (entered as positive) for input table of time versus sink fluxes, for every QRT sink in the model.

QRT is attached to IUNIT(41)

FLOW AND HEAD BOUNDARY (FHB) PACKAGE INPUT INSTRUCTIONS

Input for the FHB package is in free format, which requires each of the numbered data groups to start on a new input record. More than one record can be used for any data group and numbers within data groups must be separated by at least one space or a comma. Integer data types cannot include a decimal point. Blank spaces are not treated as zeros. A STAIRCASE option applies the boundary in a stepwise manner instead of interpolating.

FOR EACH SIMULATION

1. Data: NBDTIM NFLW NHED IFHBSS IFHBCB NFHBX1 NFHBX2 [OPTIONS]

Type: Integer Integer Integer Integer Integer Integer Integer Character

Omit data item 2 if NFHBX1=0. Input item 2 consists of one record for each of NFHBX1 auxiliary variables.

2. Data: VarName Weight

Type: Character Real

Omit data item 3 if NFHBX2=0. Input item 3 consists of one record for each of NFHBX2 auxiliary variables.

3. Data: VarName Weight

Type: Character Real

Data items 4a and 4b are required for all simulations. Include NBDTIM times in data item 4b.

4a. Data: IFHBUN CNSTM IFHBPT

Type: Integer Real Integer

4b. Data: BDTIM(NBDTIM)

Type: Real

Omit data items 5a and 5b or 5c if NFLW=0. Input item 5b or 5c consists of one set of numbers for each of NFLW cells. Each set of numbers includes layer, row, and column indices (for item 5b), node index (for item 5c), an integer auxiliary variable, and NBDTIM values of specified flow.

5a. Data: IFHBUN CNSTM IFHBPT

Type: Integer Real Integer

Omit data item 5b for unstructured grid input

5b. Data: Layer Row Column IAUX FLWRAT(NBDTIM)

Type: Integer Integer Integer Integer Real

Omit data item 5c for structured grid input

5c. Data: Node IAUX FLWRAT(NBDTIM)

Type: Integer Integer Real

Omit data items 6a and 6b if NFHBX1=0 or if NFLW=0. Include one set of data items 6a and 6b for each of NFHBX1 auxiliary variables. Input item 6b consists of one set of numbers for each of NFLW cells. Each set includes NBDTIM values of the variable.

6a. Data: IFHBUN CNSTM IFHBPT

Type: Integer Real Integer

6b. Data: AuxVar(NBDTIM)

Type: Real

Omit data items 7a and 7b or 7c if NHED=0. Input item 7b or 7c consists of one set of numbers for each of NFLW cells. Each set of numbers includes layer, row, and column indices (for item 7b), node index (for item 7c), an integer auxiliary variable, and NBDTIM values of specified head.

7a. Data: IFHBUN CNSTM IFHBPT

Type: Integer Real Integer

Omit data item 7b for unstructured grid input

7b. Data: Layer Row Column IAUX SBHED(NBDTIM)

Type: Integer Integer Integer Integer Real

Omit data item 7c for structured grid input

7c. Data: Node IAUX SBHED(NBDTIM)

Type: Integer Integer Real

Omit data items 8a and 8b if NFHBX2=0 or if NHED=0. Include one set of data items 8a and 8b for each of NFHBX2 auxiliary variables. Input item 8b consists of one set of numbers for each of NHED cells. Each set includes NBDTIM values of the variable.

8a. Data: IFHBUN CNSTM IFHBPT

Type: Integer Real Integer

8b. Data: AuxVar(NBDTIM)

Type: Real

Explanation of Variables Read by the FHB Package

NBDTIM—is the number of times at which flow and head will be specified for all selected cells.

If NBDTIM = 1, specified flow and head values will remain constant for the entire simulation.

If NBDTIM > 1, specified flow and head values will be computed for each time step using linear interpolation.

NFLW—is the number of cells at which flows will be specified.

NHED—is the number of cells at which head will be specified.

IFHBSS—is the FHB steady-state option flag. If the simulation is transient, the flag is read but not used.

For steady-state simulations, the flag controls how specified-flow, specified-head, and auxiliary-variable values will be computed for each steady-state solution.

If IFHBSS = 0, values of flow, head, and auxiliary variables will be taken at the starting time of the simulation. This results in use of the first value in arrays FLWRAT, SBHED, and AuxVar for each respective boundary cell.

If IFHBCB □□ 0, values of flow, head, and auxiliary variables will be interpolated in the same way that values are computed for transient simulations.

IFHBCB—is a flag and unit number.

If IFHBCB > 0, it is the unit number on which cell-by-cell flow terms will be recorded whenever ICBCFL is set (see McDonald and Harbaugh, 1988, chap. 4, p. 14–15).

If IFHBCB □ 0, cell-by-cell flow terms will not be recorded.

NFHBX1—is the number of auxiliary variables whose values will be computed for each time step for each specified-flow cell.

NFHBX2—is the number of auxiliary variables whose values will be computed for each time step for each specified-head cell.

OPTIONS are keywords that activate options:

STAIRCASE indicates that interpolation will not be performed on the time series for heads or fluxes, and instead, the values will be staircased, till the next time value in the table is reached. For example, if there are 3 time values in a table of time versus flux, and the time values are 0.0, 365.0, 1000.0, and if the flux values are 100, 500, 200, then the flux value of 100 is applied from 0 to 365 days, the flux value of 500 is applied from 365 to 1000 days, and a flux value of 200 is applied beyond 1000 days of the simulation.

VarName—is the name of an auxiliary variable. Name can include up to 16 characters with no embedded blank characters.

Weight—is the time-weighting factor for an auxiliary variable specifying the fraction of each time step at which the value of the variable will be interpolated. Value must be in the range from 0.0 to 1.0.

IFHBUN—is the unit number on which data lists will be read. The same or different unit numbers can be used to read lists in data items 4b, 5b, 5c, 6b, 7b, 7c, and 8b.

CNSTM—is a constant multiplier for data list BDTIM (data item 4b), FLWRAT (part of data item 5b or 5c), SBHED (part of data item 7b or 7c), and auxiliary variables in data items 6b and 8b.

IFHBPT—is a flag for printing values of data lists in items 4b, 5b, 5c, 6b, 7b, 7c, and 8b.

If IFHBPT > 0 data list read at the beginning of the simulation will be printed.

If IFHBCB < 0 data list read at the beginning of the simulation will not be printed.

BDTIM—is simulation time at which values of specified flow and (or) values of specified head will be read. NBDTIM values are required.

Layer—is the layer index of specified-flow cell (data item 5b) or specified-head cell (data item 7b).

Row—is the row index of specified-flow cell (data item 5b) or specified-head cell (data item 7b).

Column—is the column index of specified-flow cell (data item 5b) or specified-head cell (data item 7b).

Node—is the node number of specified-flow cell (data item 5c) or specified-head cell (data item 7c).

IAUX—is an integer auxiliary variable associated with each specified-flow and specified-head boundary cell. A value is read but not used in simulations of ground-water flow with MODFLOW-96. IAUX can be used by programs such as MODPATH (Pollock, 1994) to store information such as the cell face associated with the specified-flow or specified-head boundary.

FLWRAT—is volumetric rate of flow at specified-flow cells. A list of NBDTIM values must be specified for each of NFLW specified-flow cells.

AuxVar—is value of real auxiliary variable at specified-flow and specified-head cells. A list of NBDTIM values must be specified for each of NFLW specified-flow cells and for each of NHED specified-head cells.

SBHED—is an array containing NBDTIM values of the head for each specified-head cell.

RIVER (RIV) PACKAGE INPUT INSTRUCTIONS

Input to the River (RIV) Package is read from the file that has file type "RIV" in the Name File. Optional variables are shown in brackets. All variables are free format if the option “FREE” is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format.

Optional variables are used in the RIV Package to identify species concentrations for transport simulations. The concentration in the river is input to the code as an AUXILIARY variable. The name identifies the species for which the auxiliary variable is designated. For example, C01 identifies the variable as the concentration of species 1; C02 identifies the variable as the concentration of species 2; and in general, Cxx identifies the variable as the concentration of species “xx”.

The RIV package has further been modified to include the hydraulic conductivity of the grid-block on which the river sits, in the computation of total conductance between the river and the cell on which it lies. The conductance is computed as the harmonic mean of the conductance input to the RIV bottom and the conductance of half-grid block thickness of the cell from the center to the top. The option is called “**MERGE_BED_K1”.** No further input is required if this option is used.

The RIV package has been further modified to allow optional binary input of the river data which can be used for any USG-T simulation. This was specifically done to speed-up data transfer for IHM simulations which pass information back and forth between the surface-water model and the groundwater model USG-T. Binary data is accommodated by using the optional keyword “BINARY” followed by a Fortran unit number on which the binary information will be stored. The binary file should be opened with the same unit number in the NAMEFILE of the simulation as a BINARY data type. The binary file will contain information of data items 5 and 6 at every stress period, instead of using the ASCII formats in the same file. For an IHM simulation the NO-ARCHIVE file type further saves only the latest stress period information from IHM and therefore

USG-T does not advance and goes to the start of the file to read information for the next stress period.

FOR EACH SIMULATION

0. [#Text]

   Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. [***PARAMETER*** NPRIV MXL]

   This optional item must start with the word "PARAMETER".

2. MXACTR IRIVCB [Option]

3. [PARNAM PARTYP Parval NLST [***INSTANCES*** NUMINST]]

   Repeat Item 3 combined with the indicated repetitions of Item 4 NPRIV times. Items 3 and 4 are not read if NPRIV is negative or 0.

   If PARNAM is to be a time-varying parameter, the keyword "INSTANCES" and a value for NUMINST must be entered.

4a. [INSTNAM]

4b. [Layer Row Column Stage Condfact Rbot [xyz]]

   Omit Item 4b if an unstructured grid is used

4c. Node Stage Condfact Rbot [xyz]

   Omit Item 4c if a structured grid is used

   After each Item 3 for which the keyword "INSTANCES" is not entered, read Item 4b or 4c and not Item 4a.

   After each Item 3 for which the keyword "INSTANCES" is entered, read Item 4a and Item 4b or 4c for each instance.

NLST repetitions of Item 4b or 4c are required; they are read by subroutine ULSTRD. (SFAC of the ULSTRD utility subroutine applies to Condfact). The NLST repetitions of Item 4b or 4c follow each repetition of Item 4a when PARNAM is time varying.

FOR EACH STRESS PERIOD

Note that items 5 and 6 are in binary format if the BINARY option is used, and this data is presented in a separate binary file that is opened on the unit number presented with the BINARY option. The file has to be opened with the same unit number as a BINARY data format file in the simulation NAMEFILE. The binary option is specifically provided to accommodate quick data transfer for IHM simulations where surface-water and groundwater exchange information at every stress period.

5. ITMP NP

6a. Layer Row Column Stage Cond Rbot [xyz]

Omit Item 6a if an unstructured grid is used

6b. Node Stage Cond Rbot [xyz]

Omit Item 6b if a structured grid is used

ITMP repetitions of Items 6a or 6b are read by subroutine ULSTRD if ITMP > 0. (SFAC of the ULSTRD utility subroutine applies to Cond.) Items 6a or 6b are not read if ITMP is negative or 0.

7. [Pname [Iname]]

(Item 7 is repeated NP times. Item 7 is not read if NP is negative or 0. Iname is read if Pname is a time-varying parameter.)

Explanation of Variables Read by the RIV Package:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The

"#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPRIV—is the number of river parameters.

MXL—is the maximum number of river reaches that will be defined using parameters.

MXACTR—is the maximum number of river reaches in use during any stress period, including those that are defined using parameters.

IRIVCB—is a flag and a unit number.

If IRIVCB > 0, cell-by-cell flow terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control.

If IRIVCB = 0, cell-by-cell flow terms will not be written.

If IRIVCB < 0, river leakage for each reach will be written to the listing file when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control.

Option—is an optional list of character values.

"AUXILIARY abc" or "AUX abc"—defines an auxiliary variable, named "abc", which will be read for each river reach as part of Items 4 and 6. Up to 20 variables can be specified, each of which must be preceded by "AUXILIARY" or "AUX." These variables will not be used by the Ground-Water Flow Process Package, but they will be available for use by other processes. The auxiliary variable values will be read after the Rbot variable. Note that if the auxiliary variable name is "Cxx", it identifies the variable as the concentration of species "xx". Thus, $C0_1$ is concentration of species number 1, $C0_2$ is concentration of species number 2, and so forth (up to 99 species).

"NOPRINT"—specifies that lists of river reaches will not be written to the Listing File.

"MERGE_BED_K1"—specifies that the bed conductance that is specified in this file (in Cond or Condfact) is to be merged with the vertical conductance of the groundwater cell from the bottom of the river till the center of the cell, if the bottom of the river is above the cell center. This option allows for independent control of the river bed type from the vertical conductance of the cell on which it sits.

"BINARY ib"—is a keyword that specifies that all RIV data following this header line will be read by USG-T in binary format, from file that is attached to Fortran Unit "ib". This file should also be opened in the NAME file in "Binary DATA" format on the same Fortran Unit number "ib". Information in the binary file includes data for items 5 and 6 for only the last stress period if the associated binary file is opened using the "NO-ARCHIVE" keyword in the NAME file. Otherwise, by default, the data is stored and available in the binary file at every stress period, for data transfer between IHM and USG-T during a simulation. Further note that for a binary file, the variable of item 5 (ITMP) is an integer*4 variable, the node identification on data item 6 (node number for unstructured grid or layer, row, column for structured grid) are also an integer*4 variables, and the other variables of item 6 (river stage, conductance and bed elevation) are real*4 variables.

PARNAM—is the name of a parameter. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter. For the RIV Package, the only allowed parameter type is RIV, which defines values of riverbed hydraulic conductance.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NLST—is the number of river reaches in a non-time-varying parameter. For a time-varying parameter, NLST is the number of reaches in each instance.

INSTANCES—is an optional keyword that designates a parameter as time varying. The keyword is not case sensitive; that is, any combination of the same characters with different case will be equivalent. If ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, PARNAM is non-time-varying and NUMINST should not be present.

NUMINST—is the number of instances for a time-varying parameter, where each instance is a list of river reaches and associated properties. If the keyword ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, NUMINST should not be present.

INSTNAM—is the name of an instance associated with the parameter named in the corresponding Item 3. The instance name can be 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent. Instance names must be unique for a parameter, but instance names may be reused for different parameters.

Layer—is the layer number of the cell containing the river reach.

Row—is the row number of the cell containing the river reach.

Column—is the column number of the cell containing the river reach.

Node—is the node number of the model cell that contains the river reach.

Stage—is the head in the river.

Condfact—is the factor used to calculate riverbed hydraulic conductance from the parameter value. The conductance is the product of Condfact and the parameter value.

Rbot—is the elevation of the bottom of the riverbed.

[xyz]—represents the values of the auxiliary variables for a river reach that have been defined in Item 2. The values of auxiliary variables must be present in each repetition of Items 4 and 6 if they are defined in Item 2. The values must be specified in the order used to define the variables in Item 2.

ITMP—is a flag and a counter.

If ITMP < 0, non-parameter river data from the last stress period will be reused.

If ITMP ≥ 0, ITMP will be the number of non-parameter reaches read for the current stress period.

NP—is the number of parameters in use in the current stress period.

Cond—is the riverbed hydraulic conductance.

Pname—is the name of a parameter that is being used in the current stress period. NP parameter names will be read.

Iname—is an instance name that is read only if Pname is a time-varying parameter. Multiple instances of the same parameter are not allowed in a stress period.

STREAM (STR7) PACKAGE INPUT INSTRUCTIONS

Input to the modified version of the Streamflow-Routing (STR) Package is read from the file that has file type "STR" in the MODFLOW name file. Optional variables are shown in brackets. All variables are read with fixed format except as noted.

The STR7 package does not yet support solute or heat transport. **Thus, if a solute reaches a STR7 boundary, it will accumulate at the boundary and will not be let out with the water.**

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional -- "#" must be in column 1. Item 0 can be repeated multiple times.

1. [***PARAMETER*** NPSTR MXL]

This optional record is read with free format; it must start with the word "PARAMETER".

2. MXACTS NSS NTRIB NDIV ICALC CONST ISTCB1 ISTCB2

I10 I10 I10 I10 I10 F10.0 I10 I10

3. [PARNAM PARTYP Parval NLST [***INSTANCES*** NUMINST]]

Item 3 is read with free format. If PARNAM is to be a time-varying parameter, the keyword "INSTANCES" and a value for NUMINST must be entered.

4a. [INSTNAM]

Item 4a is read only if PARNAM is time varying. NUMINST repetitions of Item 4 (parts a and b) are read. After each repetition of Item 4a, NLST repetitions of Item 4b are read.

4b. [Layer Row Col Seg Reach Flow Stage Condfact Sbot Stop]

I5 I5 I5 I5 I5 F15.0 F10.0 F10.0 F10.0 F10.0

NLST repetitions of Item 4b are required. The NLST repetitions of Item 4b follow each repetition of Item 4a when PARNAM is time varying. Repeat Items 3 and 4 for each of NPSTR parameters.

Omit Item 4b if an unstructured grid is used

4c. [Node Seg Reach Flow Stage Condfact Sbot Stop]

I10 I10 I10 F10.0 F10.0 F10.0 F10.0 F10.0

NLST repetitions of Item 4c are required. The NLST repetitions of Item 4c follow each repetition of Item 4a when PARNAM is time varying. Repeat Items 3 and 4 for each of NPSTR parameters.

Omit Item 4c if a structured grid is used

FOR EACH STRESS PERIOD

5. ITMP IRDFLG IPTFLG

I10 I10 I10

6a. Layer Row Col Seg Reach Flow Stage Cond Sbot Stop

I5 I5 I5 I5 I5 F15.0 F10.0 F10.0 F10.0 F10.0

Omit Item 6a if an unstructured grid is used

6b. Node Seg Reach Flow Stage Cond Sbot Stop

I10 I10 I10 F10.0 F10.0 F10.0 F10.0 F10.0

Omit Item 6b if a structured grid is used

Item 6a or 6b is repeated ITMP times if NPSTR=0. If ITMP<0, Item 6a or 6b records are used from the previous stress period.

7. [Pname [Iname]]

Item 7 is repeated ITMP times if NPSTR>0. Free format is used. Iname is read if Pname is a time-varying parameter.

[Note that either Item 6 or Item 7 may be read, but not both.]

8. Width Slope Rough

F10.0 F10.0 F10.0

Item 8 is read only if ICALC > 0, in which case Item 8 is repeated for every stream reach. The records must be is the same order as the stream reaches.

9. Itrib(NTRIB)

10I5

Item 9 is read only if NTRIB > 0, in which case Item 9 is repeated NSS times in sequential order of the segments. Each record contains NTRIB values.

10. Iupseg

I10

Item 10 is read only if NDIV>0, in which case Item 10 is repeated NSS times in sequential order of the segments.

Explanation of Variables Read by the STR Package:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Text is printed when the file is read.

NPSTR—is the number of stream parameters that will be defined.

MXL—is the maximum number of stream reaches that will be defined using parameters. MXL must equal or exceed the sum of NLST x NUMINST for all parameters.

MXACTS—is the maximum number of stream reaches that will be in use during any stress period. MXACTS includes reaches that are defined using parameters as well as reaches that are defined without using parameters.

NSS—is the number of stream segments

NTRIB—is the number of stream tributaries that can connect to one segment. The program is currently dimensioned so that NTRIB cannot exceed 10.

NDIV—is a flag, which when positive, specifies that diversions from segments are to be simulated.

ICALC—is a flag, which when positive, specifies that stream stages in reaches are to be calculated.

CONST—is a constant value used in calculating stream stage in reaches. It is specified whenever ICALC is greater than 0. This constant is 1.486 for flow units of cubic feet per second and 1.0 for units of cubic meters per second. The constant must be multiplied by 86,400 when using time units of days in the simulation.

ISTCB1—is a flag and a unit number for the option to write seepage between the stream reaches and model cells into the list file or an unformatted (binary) file.

If ISTCB1>0, it is the unit number to which seepage between each stream reach and the corresponding model cell will be saved whenever the variable ICBCFL in the Output Control Option is set.

If ISTCB1=0, seepage between each stream reach and the corresponding model cell will not be written into any file.

If ISTCB1<0, streamflow for each reach and seepage between each stream reach and the corresponding models cell will be written into the LIST file whenever the variable ICBCFL in the Output Control Option is set.

ISTCB2—is a flag and a unit number for the option to store streamflow out of each reach in an unformatted (binary) file.

If ISTCB2 > 0, it is the unit number to which streamflow in each stream reach will be saved whenever the variable ICBCFL in the Output Control Option is set.
If ISTCB2 ≤ 0, streamflow in each stream reach will not be stored in a disk file.

PARNAM—is the name of a parameter. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter to be defined. For the STR Package, the only allowed parameter type is STR, which defines values of streambed conductance.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NLST—is the number of stream reaches that are included in each instance defined for the parameter.

INSTANCES—is an optional keyword that designates a parameter as time varying. The keyword is case-insensitive; that is, it may be entered in any combination of upper- and lower-case letters. If ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, PARNAM is non-time-varying and NUMINST should not be present.

NUMINST—is the number of instances that are included in the definition of a time-varying parameter, where each instance is a list of stream reaches and associated properties. If the keyword ***INSTANCES*** is present, NUMINST must be present. If the keyword ***INSTANCES*** is absent, NUMINST should not be present.

INSTNAM—is the name of an instance associated with the parameter PARNAM specified in the corresponding Item 3. The name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent. Names entered for INSTNAM must be unique for any given parameter, but names may be reused for instances associated with different parameters.

Layer—is the layer number of the model cell containing the stream reach.

Row—is the row number of the model cell containing the stream reach.

Col—is the column number of the model cell containing the stream reach.

Node—is the node number of the model cell containing the stream reach.

Seg—is a number assigned to a group of reaches. Segments must be numbered in downstream order and are read into the program in sequential order.

Reach—is a sequential number in a segment that begins with 1 for the farthest upstream reach and continues in downstream order to the last reach in the segment. Reaches must be read in sequentially because the order in which reaches are read determines the order of connection.

Flow—is the streamflow entering a segment. This value is used only for the first reach of each segment. The value should be specified as either 0 or blank when the reach number (Reach) is not 1. When the inflow to the first reach of a segment is the sum of the outflow from upstream tributary segments, Flow should be specified as -1. When the segment is a diversion, the Flow for the first reach is the amount to divert; however, there will be no diversion if the segment from which the diversion is obtained contains less than the value of Flow.

Stage—is the stream stage. The value of Stage is not used if ICALC>0.

Condfact—is the factor used to calculate streambed hydraulic conductance from the parameter value. The conductance is the product of Condfact and the parameter value.

Sbot—is the elevation of the bottom of the streambed.

Stop—is the elevation of the top of the streambed. The value of Stop is used if the option to calculate stream stage is active (ICALC>0) or when the streambed has zero flow.

ITMP—is a flag and a counter. Its meaning depends on whether or not stream parameters are being used.

If STR parameters are being used (NPSTR>0), ITMP is the number of stream parameters being used in the current stress period.

IF STR parameters are not being used (NPSTR=0), ITMP is the number of stream reaches for which data will be read in the current stress period. If ITMP < 0, STR data from the preceding stress period will be reused.

IRDFLG—is a flag, which when positive, suppresses printing of the stream input data for a stress period. The input data are printed if IRDFLG is 0 and ICBCFL in the Output Control Option is set.

IPTFLG—is a flag, which when positive, suppresses printing of stream results for a stress period. Results are printed if IPTFLG is 0, ICBCFL in the Output Control Option is set, and ISTCB1 < 0.

Cond—is the streambed hydraulic conductance.

Pname—is the name of a parameter that is being used in the current stress period. ITMP parameter names will be read. They must be specified in an order that meets the downstream ordering requirements for Seg and Reach.

Iname—is an instance name that is read only if Pname is a time-varying parameter. Multiple instances of the same time-varying parameter are not allowed in a stress period.

Width—is the width of the stream channel. It is read only when stream stage is calculated (ICALC>0).

Slope—is the slope of the stream channel. It is read only when stream stage is calculated (ICALC>0).

Rough—is Manning's roughness coefficient. It is read only when stream stage is calculated (ICALC>0).

Itrib—contains the segment number for each tributary that flows into a segment. NTRIB values are read for each segment. Unused values of Itrib should be set to 0. Itrib records are read only when NTRIB>0.

Iupseg—is the number of the upstream segment from which water is diverted. If the segment is not a diversion, Iupseg should be specified as 0. Iupseg records are read only when NDIV>0.

STREAMFLOW-ROUTING (SFR2) PACKAGE WITH UNSATURATED FLOW BENEATH STREAMS.

MODFLOW Name File

The Streamflow-Routing Package is activated automatically by including a record in the MODFLOW name file using the file type (Ftype) “SFR” to indicate that relevant calculations are to be made in the model and to specify the related input data file. The user can optionally specify that stream gages and monitoring stations are to be represented at one or more locations along a stream channel by including a record in the MODFLOW name file using the file type (Ftype) “GAGE” that specifies the relevant input data file giving locations of gages. The modifications in SFR2 do not require any changes to the data input for SFR1. SFR2 is compatible with MODFLOW-2000 (Harbaugh and others, 2000), but not with earlier versions of MODFLOW.

The SFR2 package does not support solute or heat transport. **Thus, if a solute reaches a SFR2 boundary, it will accumulate at the boundary and will not be let out with the water.**

Input Data Instructions

The modification of SFR2 to simulate unsaturated flow relies on the specific yield values as specified in the Layer Property Flow (LPF) Package or the Block-Centered Flow (BCF) Package. Thus, the option for unsaturated flow beneath streams is only available when either LPF or BCF is used in the simulation. When the option to use vertical hydraulic conductivity in the LPF Package is specified, the layer(s) that contain cells where unsaturated flow will be simulated must be specified as convertible. That is, the variable LAYTYP specified in LPF must not be equal to zero, otherwise the model will print an error and stop execution.

Additional variables that must be specified to define hydraulic properties of the unsaturated zone are all included within the SFR2 input file. All values are entered in as free format. Data input for SFR1 works without modification if unsaturated flow is not simulated. Parameters can be used to define streambed hydraulic conductivity only when data input follows the SFR1 input structure (Prudic and others, 2004). The calculation of sensitivities for, or estimation of, parameters using the Sensitivity Process are not supported by SFR1 nor SFR2. Additionally, the Ground-Water Transport Process is only available using the original SFR1 input structure and is currently not available when simulating unsaturated flow beneath streams.

For each simulation, the first record in the SFR2 input file must read:

FOR EACH SIMULATION

0. [#Text] Text A character variable (up to 199 characters) that is printed when the file is read. The "#" character must be in column 1, and, accordingly, the variable starts in column 2. Any characters can be included in Text.

Note 1: Item 0 can be repeated multiple times.

1a. Data: {REACHINPUT TRANSROUTE}

REACHINPUT An optional character variable that is a flag to change the default format for entering reach and segment data input and to simulate unsaturated flow beneath streams. When REACHINPUT is specified, optional variable ISFROPT must be specified in item 1c; optional variables NSTRAIL, ISUZN, and NSFRSETS also must be specified if ISFROPT>0.

TRANSROUTE An optional character variable that is a flag to indicate that transient streamflow routing is active. When TRANSROUTE is specified, optional variables IRTFLG, NUMTIM, WEIGHT, and FLWTOL also must be specified in Item 1c.

1b. Data: {TABFILES NUMTAB MAXVAL}

TABFILES An optional character variable that is a flag to indicate that inflows to one or more stream segments will be specified with tabular inflow files.

NUMTAB An integer value equal to the number of tabular inflow files that will be read if TABFILES is specified. A separate input file is required for each segment that receives specified inflow. Thus, the maximum value of NUMTAB that can be specified is equal to the total number of segments specified in Item 1c with variables NSS. The name (Fname) and unit number (Nunit) of each tabular file must be specified in the MODFLOW-USG Name File using tile type (Ftype) DATA.

MAXVAL An integer value equal to the largest number of rows of specified inflows for any of the tabular inflow files if TABFILES is specified. MAXVAL is used for memory allocation. For example, if there are two tabular inflow files and the files contain

100 and 200 inflow values, respectively, then MAXVAL would be specified as 200.

1c. Data: NSTRM NSS NSFRPAR NPARSEG CONST DLEAK ISTCB1 ISTCB2 {ISFROPT} {NSTRAIL} {ISUZN} {NSFRSETS} {IRTFLG} {NUMTIM} {WEIGHT} {FLWTOL}

NSTRM — An integer value equal to the number of stream reaches (finite-difference cells) that are active during the simulation. The value of NSTRM also represents the number of lines of data to be included in Item 2, described below.

NSS — An integer value equal to the number of stream segments (consisting of one or more reaches) that are used to define the complete stream network. The value of NSS represents the number of segments that must be defined through a combination of parameters and repetitions of Item 6 every stress period.

NSFRPAR — An integer value equal to the number of stream parameters (associated with one or more segments) to be defined. This variable must be zero when NSTRM is negative.

NPARSEG — An integer value equal to (or exceeding) the number of stream-segment definitions associated with all parameters. This number can be more than the total number of segments (NSS) in the stream network because the same segment can be defined in multiple parameters, and because parameters can be time-varying. NPARSEG must equal or exceed the sum of NLST × N for all parameters, where N is the greater of 1 and NUMINST; that is, NPARSEG must equal or exceed the total number of repetitions of item 4b. This variable must be zero when NSTRM is negative.

CONST — A real value (or conversion factor) used in calculating stream depth for stream reach. If stream depth is not calculated using Manning's equation for any stream segment (that is, ICALC does not equal 1 or 2), then a value of zero can be entered. If Manning's equation is used, a constant of 1.486 is used for flow units of cubic feet per second, and a constant of 1.0 is used for units of cubic meters per second. The constant must be multiplied by 86,400 when using time units of days in the simulation. An explanation of time units used in MODFLOW is given by Harbaugh and others (2000, p. 10.)

DLEAK A real value equal to the tolerance level of stream depth used in computing leakage between each stream reach and active model cell. Value is in units of length. Usually a value of 0.0001 is sufficient when units of feet or meters are used in model.

ISTCB1 An integer value used as a flag for writing stream-aquifer leakage values. If ISTCB1 > 0, it is the unit number to which unformatted leakage between each stream reach and corresponding model cell will be saved to a file whenever the cell-by-cell budget has been specified in Output Control (see Harbaugh and others, 2000, pages 52-55). If ISTCB1 = 0, leakage values will not be printed or saved. If ISTCB1 < 0, all information on inflows and outflows from each reach; on stream depth, width, and streambed conductance; and on head difference and gradient across the streambed will be printed in the main listing file whenever a cell-by-cell budget has been specified in Output Control.

ISTCB2 An integer value used as a flag for writing to a separate formatted file all information on inflows and outflows from each reach; on stream depth, width, and streambed conductance; and on head difference and gradient across the streambed. If ISTCB2 > 0, then ISTCB2 also represents the unit number to which all information for each stream reach will be saved to a separate file when a cell-by-cell budget has been specified in Output Control. If ISTCB2 < 0, it is the unit number to which unformatted streamflow out of each reach will be saved to a file whenever the cell-by-cell budget has been specified in Output Control.

If keyword REACHINPUT has been specified:

ISFROPT An integer value that defines the input structure

1 No vertical unsaturated flow beneath streams. Streambed elevation, stream slope, streambed thickness, and streambed hydraulic conductivity are read for each reach only once at the beginning of the simulation.

2 Streambed and unsaturated-zone properties are read for each reach only once at the beginning of the simulation except saturated vertical hydraulic conductivity for the unsaturated zone is the same as the vertical hydraulic conductivity of the corresponding layer in LPF and is not read in separately.

3 Same as 2 except saturated vertical hydraulic conductivity for the unsaturated zone is read for each reach.

4 Streambed and unsaturated-zone properties are read for the beginning and end of each stream segment. Streambed properties can vary each stress period. Saturated vertical hydraulic conductivity for the unsaturated zone is the same as the vertical hydraulic conductivity of the corresponding layer in LPF and is not read in separately.

5 Same as 4 except saturated vertical hydraulic conductivity for the unsaturated zone is read for each segment at the beginning of the first stress period only.

Note 2: If BCF is used and unsaturated flow is active then ISFROPT must equal 3 or 5.

When ISFROPT is greater than 1, read the following variables:

NSTRAIL An integer value that is the number of trailing wave increments used to represent a trailing wave. Trailing waves are used to represent a decrease in the surface infiltration rate. The value can be increased to improve mass balance in the unsaturated zone. Values between 10 and 20 work well, although, for large problems we recommend fewer trailing waves (10) due to memory and computational requirements. Please see Smith (1983) for further details.

ISUZN An integer value that is the maximum number of vertical cells used to the define the unsaturated zone beneath a stream reach. If ICALC is 1 for all segments then ISUZN should be set to 1.

NSFRSETS An integer value that is the maximum number of different sets of trailing waves used to allocate arrays. Arrays are allocated by multiplying NSTRAIL by NSFRSETS. A value of 30 is sufficient for problems where the stream depth varies often.

If keyword TRANSROUTE has been specified:

IRTFLG An integer value that indicates the method of transient streamflow routing. IRTFLG must be specified if TRANSROUTE has been specified. Currently, the only routing method available is the kinematic-wave equation approach (see USGS Techniques and Methods 6-D1, p. 68-69). Enter IRTFLG=1, if

streamflow will be routed using the kinematic-wave equation; otherwise, IRTFLG should be specified as 0 (steady flow).

If IRTFLG = 1:

NUMTIM An integer value equal to the number of sub time steps used to route streamflow. The time step that will be used to route streamflow will be equal to the MODFLOW-2005 time step divided by NUMTIM.

WEIGHT A real number equal to the time weighting factor used to calculate the change in channel storage. WEIGHT has a value between 0.5 and 1. Refer to equation 83 in USGS Techniques and Methods 6-D1 for further details.

FLWTOL A real number equal to the streamflow tolerance for convergence of the kinematic wave equation used for transient streamflow routing. A value of 0.00003 cubic meters per second has been used successfully in test simulations (and would need to be converted to whatever units are being used in the particular simulation).

Note 3: The first two variables (NSTRM and NSS) are used for dimensioning arrays, and must be equal to the actual number of stream reaches defined in Item 2 and the number of segments that define the complete stream network, respectively.

Note 4: SFR2 differs from the Stream (STR1) Package (Prudic, 1989) because the new package solves for stream depth at the midpoint of each reach instead of at the beginning of the reach. To solve for depth at the midpoint of each reach, like SFR1, SFR2 uses Newton's iterative method and consequently, a tolerance (DLEAK) is used for stopping the iterative process.

ONE RECORD FOR EACH STREAM REACH:

2a. Data: KRCH IRCH JRCH ISEG IREACH RCHLEN {STRTOP} {SLOPE} {STRTHICK} {STRHC1} {THTS} {THTI} {EPS} {UHC}

Omit Item 2a if an unstructured grid is used

2b. Data: NRCH ISEG IREACH RCHLEN {STRTOP} {SLOPE} {STRTHICK} {STRHC1} {THTS} {THTI} {EPS} {UHC}

Omit Item 2b if a structured grid is used

KRCH	An integer value equal to the layer number of the cell containing the stream reach.
IRCH	An integer value equal to the row number of the cell containing the stream reach.
JRCH	An integer value equal to the column number of the cell containing the stream reach.
NRCH	An integer value equal to the node number of the cell containing the stream reach.
ISEG	An integer value equal to the number of stream segment in which this reach is located. Stream segments contain one or more reaches and are assumed to have uniform or linearly varying characteristics.
IREACH	An integer value equal to the sequential number in a stream segment of this reach (where a reach corresponds to a single cell in the model). Numbering of reaches in a segment begins with 1 for the farthest upstream reach and continues in downstream order to the last reach of the segment.
RCHLEN	A real number equal to the length of channel of the stream reach within this model cell. The length of a stream reach can exceed the model cell dimensions because of the meandering nature of many streams. The length is used to calculate the streambed conductance for this reach. Also, the sum of the lengths of all stream reaches within a segment is used to calculate the average slope of the channel for the segment and subsequently other values, such as the elevation of the streambed and stream stage.
STRTOP	A real number equal to the top elevation of the streambed. This variable is read when ISFROPT is 1, 2, or 3.
SLOPE	A real number equal to the stream slope across the reach. This variable is read when ISFROPT is 1, 2, or 3. Slope must be greater than zero.
STRTHICK	A real number equal to the thickness of the streambed. This variable is read when ISFROPT is 1, 2, or 3.

STRHC1 A real number equal to the hydraulic conductivity of the streambed. This variable is read when ISFROPT is 1, 2, or 3.

THTS A real number equal to the saturated volumetric water content in the unsaturated zone. This variable is read when ISFROPT is 2 or 3.

THTI A real number equal to the initial volumetric water content. THTI must be less than or equal to THTS and greater than or equal to THTS minus the specific yield defined in LPF or BCF. This variable is read when ISFROPT is 2 or 3.

EPS A real number equal to the Brooks-Corey exponent used in the relation between water content and hydraulic conductivity within the unsaturated zone (Brooks and Corey, 1966). This variable is read when ISFROPT is 2 or 3.

UHC A real number equal to the vertical saturated hydraulic conductivity of the unsaturated zone. This variable is necessary when using BCF, whereas it is optional when using LPF. This variable is read when ISFROPT is 3.

Note 5: Records are read in sequential order from upstream to downstream, first by segments, and then sequentially by reaches. Segments should be numbered in downstream order but this is not necessary. However, if the segments are not numbered in downstream order, the inflows and outflows from each segment will still be computed but the computed inflows into a segment from upstream tributary streams having a higher segment number will be from the previous iteration. Reaches must be listed and read in sequentially because the order determines the connections of inflows and outflows within a stream segment.

Note 6: The stream network is assumed to remain fixed geometrically over the duration of a simulation. The active part of the stream network, however, can be made to vary over time by making selected stream segments inactive for selected stress periods. This would be implemented by setting the streambed hydraulic conductivity, segment inflow, overland runoff, and direct precipitation to zero for the inactive segments in Items 4 or 6 for the specific stress periods when they are known to be inactive or dry.

Note 7: If the model cell corresponding to a stream reach is inactive, the program will search for the uppermost active cell in the vertical column to apply the leakage. If there are no active cells or if the cell is a constant head, no interaction is allowed and flow in the reach is passed to the next reach.

Note 8: When STRTOP, SLOPE, STRTHICK, and STRHC1 are specified for each reach, the variables are not read using Items 6b or 6c.

Note 9: The residual water content for each cell is not specified by the user because it is calculated based on the specified saturated water content minus the specific yield of the active model cell corresponding to the stream reach. The calculation is performed internally to assure continuity between unsaturated and saturated zone storage.

Note 10: Although unsaturated flow variables will not be used for reaches that are designated as ICALC = 0, 3, and 4 within the segment information, values must be included for all reaches when ISFROPT = 2 or 3. Dummy values may be used for reaches that are designated as ICALC = 0, 3, and 4.

When NSFRPAR = 0, skip Items 3**and** 4**and enter all stream segment data using Items** 5**and 6; and**

When NSFRPAR > 0, Items 3**and** 4**are repeated NSFRPAR times:**

3. Data: PARNAM PARTYP Parval NLST [***INSTANCES*** NUMINST]

PARNAM A set of characters used to name a parameter to be defined. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different cases will be equivalent.

PARTYP Type of parameter to be defined. For the SFR2 Package, the only allowed parameter type is SFR, which defines values of the streambed hydraulic conductivity.

Parval A real number that is a parameter value that may be overridden by a value in the Sensitivity Process input file when ISENALL in that file is less than zero.

NLST An integer value that is the number of stream segments associated with this parameter (this value also indicates how many times Item 4 is repeated in the next block of input data).

INSTANCES An optional keyword that designates a parameter as time varying. The keyword is case-insensitive; that is, it may be entered in any combination of upper- and lower-case letters. If ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, PARNAM is non-time-varying and NUMINST should not be present.

NUMINST An integer value that is the number of instances that are included in the definition of a time-varying parameter, where each instance is a sequence of Item 4 (Parts 4b through 4g) defining reaches and associated properties. If the keyword ***INSTANCES*** is present, NUMINST must be present and must be at least 1. If the keyword ***INSTANCES*** is absent, NUMINST should not be present.

When PARNAM is not time-varying, Part 4a is not read, and Parts 4b through 4g are read sequentially for each of NLST stream segments; and

When PARNAM is time-varying, NUMINST instances are read. For each instance, Part 4a is read, and then Parts 4b through 4g are read sequentially for each of NLST stream segments (see notes 11 and 12):

4a. Data: {INSTNAM}

INSTNAM The name of an instance associated with the parameter PARNAM specified in the corresponding Item 3 (INSTNAM is read only if PARNAM is time-varying). The name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent. Names entered for INSTNAM must be unique for any given parameter, but names may be reused for instances associated with different parameters.

4b. Data: NSEG ICALC OUTSEG IUPSEG {IPRIOR} {NSTRPTS} FLOW RUNOFF ETSW PPTSW {ROUGHCH} {ROUGHBK} {CDPTH} {FDPTH} {AWDTH} {BWDTH}

NSEG An integer value of the stream segment for which information is given to identify inflow, outflow, and computation of stream depth.

ICALC An integer value used to indicate method used to calculate stream depth in this segment.

- If ICALC ≤ 0, stream depth in each reach is specified at the beginning of a stress period and remains unchanged unless flow at the midpoint of a reach is zero, then depth is set to zero in that reach. No unsaturated flow is allowed.
- If ICALC > 0, stream depth is calculated and updated each iteration of the MODFLOW solver within a time step.
- If ICALC = 1, stream depth is calculated using Manning's equation and assuming a wide rectangular channel. Unsaturated flow is simulated when ISFROPT > 1.
- If ICALC = 2, stream depth is calculated using Manning's equation and assuming an eight-point channel cross section for each segment (which allows for the computation of a wetted

perimeter and for changing hydraulic conductance of the streambed in relation to changes in flow). Unsaturated flow is simulated when ISFROPT > 1.

• If ICALC = 3, stream depth and width are calculated using a power function relating each to streamflow (Q) using equations 8 and 9 where —DEPTH(y) = CDPTH × QFDPTH and WIDTH(w) = AWDTH × QBWDTH. No unsaturated flow is allowed.

• If ICALC = 4, stream depth and width are calculated using a table relating streamflow to depth and width (the table is defined in Part 4f). No unsaturated flow is allowed.

OUTSEG An integer value of the downstream stream segment that receives tributary inflow from the last downstream reach of this segment. If this segment (identified by NSEG) does not feed (or discharge into) another downstream (tributary) segment, then enter a value of "0" for this variable. If the segment ends within the modeled grid and OUTSEG = 0, outflow from the segment is not routed anywhere and is no longer part of the stream network. One may wish to use this if all flow in the stream gets diverted into a lined canal or into a pipe. If the flow out of this segment discharges into a lake, set OUTSEG equal to the negative value of the lake identification number (where the minus sign is used as a flag to tell the model that flow enters a lake rather than a tributary stream segment).

IUPSEG An integer value of the upstream segment from which water is diverted (or withdrawn) to supply inflow to this stream segment if this segment originates as a diversion from an upstream segment. If the source of a stream segment is discharge from a lake, set IUPSEG equal to the negative value of the lake identification number (where the minus sign is used as a flag to tell the model that streamflow into this segment is derived from lake outflow rather than a stream segment). If this stream segment (identified by NSEG) does not receive inflow as a diversion from an upstream segment, then set IUPSEG = 0.

IPRIOR An integer value that only is specified if IUPSEG > 0 (do not specify a value in this field if IUPSEG = 0 or IUPSEG < 0). IPRIOR defines the prioritization system for diversion, such as when insufficient water is available to meet all

diversion stipulations, and is used in conjunction with the value of FLOW (specified below).

• When IPRIOR = 0, then if the specified diversion flow (FLOW) is greater than the flow available in the stream segment from which the diversion is made, the diversion is reduced to the amount available, which will leave no flow available for tributary flow into a downstream tributary of segment IUPSEG.

• When IPRIOR = -1, then if the specified diversion flow (FLOW) is greater than the flow available in the stream segment from which the diversion is made, no water is diverted from the stream. This approach assumes that once flow in the stream is sufficiently low, diversions from the stream cease, and is the "priority" algorithm that originally was programmed into the STR1 Package (Prudic, 1989).

• When IPRIOR = -2, then the amount of the diversion is computed asa fraction of the available flow in segment IUPSEG; in this case, $0.0 \leq FLOW \leq 1.0$.

• When IPRIOR = -3, then a diversion is made only if the streamflow leaving segment IUPSEG exceeds the value of FLOW. If this occurs, then the quantity of water diverted is the excess flow and the quantity that flows from the last reach of segment IUPSEG into its downstream tributary (OUTSEG) is equal to FLOW. This represents a flood-control type of diversion, as described by Danskin and Hanson (2002).

NSTRPTS An integer value specified only when ICALC = 4. It is used to dimension a table relating streamflow with stream depth and width as specified in Items 4e and 6e. NSTRPTS must be at least 2 but not more than 50. If the table exceeds 3 × 50 (for streamflow, stream depth, and width) values, then MAXPTS in the allocation subroutine GWF1SFR1ALP will need to be increased from 3 × 50 to 3 × (the desired maximum value).

FLOW A real number that is the streamflow (in units of volume per time) entering or leaving the upstream end of a stream segment (that is, into the first reach).

• If the stream is a headwater stream, FLOW defines the total inflow to the first reach of the segment. The value can be any number ≥ 0.

• If the stream is a tributary stream, FLOW defines additional specified inflow to or withdrawal from the first reach of the segment (that is, in addition to the discharge from the upstream segment of which this is a tributary). This additional flow does not interact with the ground-water system. For example, a positive number might be used to represent direct outflow into a stream from a sewage treatment plant, whereas a negative number might be used to represent pumpage directly from a stream into an intake pipe for a municipal water treatment plant. (Also see additional explanatory notes below.)

• If the stream is a diversionary stream, and the diversion is from another stream segment, FLOW defines the streamflow diverted from the last reach of stream segment IUPSEG into the first reach of this segment. The diversion is computed or adjusted according to the value of IPRIOR.

• If the stream is a diversionary stream, and the diversion is from a lake, FLOW defines a fixed rate of discharge diverted from the lake into the first reach of this stream segment (unless the lake goes dry) and flow from the lake is not dependent on the value of ICALC. However, if FLOW = 0, then the lake outflow into the first reach of this segment will be calculated on the basis of lake stage relative to the top of the streambed for the first reach using one of the methods defined by ICALC.

RUNOFF A real number that is the volumetric rate of the diffuse overland runoff that enters the stream segment (in units of volume per time). The specified rate is apportioned to each reach of the segment in direct relation to the fraction of the total length of the stream channel in the segment that is present in each reach.

ETSW A real number that is the volumetric rate per unit area of water removed by evapotranspiration directly from the stream channel (in units of length per time). ETSW is defined as a positive value.

PPTSW A real number that is the volumetric rate per unit area of water added by precipitation directly on the stream channel (in units of length per time).

ROUGHCH A real number that is Manning's roughness coefficient for the channel in all reaches in this segment. This variable is only specified if ICALC = 1 or 2.

ROUGHBK A real number that is Manning's roughness coefficient for the overbank areas in all reaches in this segment. This variable is only specified if ICALC = 2.

CDPTH A real number that is the coefficient used in the equation: (DEPTH = CDPTH × QFDPTH) that relates stream depth in all reaches in this segment to streamflow. This variable is only specified if ICALC = 3.

FDPTH A real number that is the coefficient used in the equation:(DEPTH = CDPTH × QFDPTH) that relates stream depth in all reaches in this segment to streamflow. This variable is only specified if ICALC = 3.

AWDTH A real number that is the coefficient used in the equation:(WIDTH = AWDTH × QBWDTH) that relates stream width in all reaches in this segment to streamflow. This variable is only specified if ICALC = 3.

BWDTH A real number that is the coefficient used in the equation:(WIDTH = AWDTH × QBWDTH) that relates stream width in all reaches in this segment to streamflow. This variable is only specified if ICALC = 3.

4c. Data: Hc1fact THICKM1 ELEVUP {WIDTH1} {DEPTH1}

Hc1fact A real number that is a factor used to calculate hydraulic conductivity of the streambed at the upstream end of this segment from the parameter value (in units of length per time).

THICKM1 A real number that is the thickness of streambed material at the upstream end of this segment (in units of length).

ELEVUP A real number that is the elevation of the top of the streambed at the upstream end of this segment (in units of length).

WIDTH1 A real number that is the average width of the stream channel at the upstream end of this segment (in units of length). This variable is only specified if ICALC $\leq$ 1.

DEPTH1 A real number that is the average depth of water in the channel at the upstream end of this segment (units of length). This variable is only specified if ICALC = 0, in which case the stream stage in a reach is assumed to equal the elevation of the top of the streambed plus the depth of water.

4d. Data: Hc2fact THICKM2 ELEVDN {WIDTH2} {DEPTH2}

Hc2fact — A real number that is the factor used to calculate hydraulic conductivity of the streambed at the downstream end of this segment from the parameter value (units of length per time).

THICKM2 — A real number that is the thickness of streambed material at the downstream end of this segment (units of length).

ELEVDN — A real number that is the elevation of the top of the streambed at the downstream end of this segment (units of length).

WIDTH2 — A real number that is the average width of the stream channel at the downstream end of this segment (units of length). This variable is only specified if ICALC $\leq$ 1.

DEPTH2 — A real number that is the average depth of water in the channel at the downstream end of this segment (units of length). This variable is only specified if ICALC = 0, in which case the stream stage in a reach is assumed to equal the elevation of the top of the streambed plus the depth of water.

If ICALC = 2:

4e. Data: XCPT1 XCPT2 **...** XCPT8
Data: ZCPT1 ZCPT2 **...** ZCPT8

XCPT*i* — A real number that is the distance relative to the left bank of the stream channel (when looking downstream) for the eight points (XCPT1 through XCPT8) used to describe the geometry of this segment of the stream channel. By definition, location XCPT1 represents the left edge of the channel cross section, and its value should be set equal to 0.0; values XCPT2 through XCPT8 should equal to or be greater than the previous distance.

ZCPT*i* — A real number that is the height relative to the top of the lowest elevation of the streambed (thalweg). One value (ZCPT1 through ZCPT8) is needed for each of the eight horizontal distances defined by XCPT*i*. The location of the thalweg (set equal to 0.0) can be any location from XCPT2 through XCPT7.

If ICALC = 4:

4f. Data: FLOWTAB(1) FLOWTAB(2) … FLOWTAB(NSTRPTS)

Data: DPTHTAB(1) DPTHTAB(2) … DPTHTAB(NSTRPTS)
Data: WDTHTAB(1) WDTHTAB(2) … WDTHTAB(NSTRPTS)

FLOWTAB A real number that is the streamflow (units of volume per time) related to a given depth and width. One value is needed for each streamflow that has a corresponding value of depth and width up to the total number of values used to define the table—FLOWTAB(1) through FLOWTAB(NSTRPTS). NSTRPTS is defined in Part 4b.

DPTHTAB A real number that is the average depth (units of length) corresponding to a given flow. The number and order of values, DPTHTAB(1)through DPTHTAB(NSTRPTS)must coincide with the streamflow values (FLOWTAB)listed on the line immediately preceding.

WDTHTAB A real number that is the stream width (units of length) corresponding to a given flow. The number and order of values, WDTHTAB(1)through WDTHTAB(NSTRPTS), must coincide with the streamflow values (FLOWTAB) listed on first line in Part 4f.

Note 11: Item 4, Parts 4b through 4g must be completed sequentially for each of the NLST stream segments; that is, Parts 4b through 4g for one stream segment must be entered before Parts 4b through 4g of the next stream segment. However, the data for stream segments need not be entered sequentially by stream segment number. For example, data for stream segment 2 can be entered before data for stream segment 1.

Note 12: When the defined parameter (PARNAM) is not time-varying, Item 4, Part 4a is omitted, and each stream segment controlled by parameter PARNAM is defined by one sequence of Parts 4b through 4g. When the defined parameter (PARNAM) is time-varying, Item 4, Parts 4a through 4g must be completed for each of NUMINST instances. For each instance, Part 4a is defined followed by Parts 4b through 4g for each of the NLST stream segments associated with that instance. For example, NUMINST = 2, NLST = 3, ICALC = 1, the sequence of records for Item 4 would be: 4a, 4b, 4c, 4d, 4b, 4c, 4d, 4b, 4c, 4d, 4a, 4b, 4c, 4d, 4b, 4c, 4d, 4b, 4c, and 4d.

Note 13: Record 4b will contain 8 to 13 variables; depending on the values of ICALC and IUPSEG. (ICALC determines how stream depth is to be calculated; when ICALC is 1 or 2, depth is calculated using Manning's equation, which, in turn, requires a channel roughness

coefficient (ICALC = 1) or a channel and bank roughness coefficient (ICALC = 2). Similarly, Parts 4c and 4d will include 3 to 5 values.

Note 14: A stream segment that receives inflow from upstream segments is allowed to have as many as ten upstream segments feeding it, as defined by the respective values of OUTSEG in Part 4b.

Note 15: Stream properties and stresses defined in Parts 4b are assumed constant and uniform within a single stream segment. Additionally, hydraulic conductivity, streambed thickness, elevation of top of streambed, stream width, and stream depth may vary smoothly and linearly within a single stream segment. For these variables, data values at the upstream end of the segment are described in Part 4c and data values at the downstream end of the segment are described in Part 4d. Values of these variables for individual reaches of a segment are estimated using linear interpolation. To make any variable the same throughout the segment, simply specify equal values in Parts 4c and 4d. The two elevations in Parts 4c and 4d are used in conjunction with the total length of the stream segment (calculated from RCHLEN given for each reach in Item 2) to compute the slope of the stream and the elevations for any intermediate reaches. The streambed thickness is subtracted from the top of streambed elevations to calculate the elevations of the bottom of the streambed (used in calculations of leakage).

Note 16: If Part 4e is included (for ICALC = 2), it is assumed that the cross-sectional geometry defined by these data is the same over the entire length of the segment. Similarly, if Part 4f is included (for ICALC = 4), it is assumed the tabulated relation between streamflow and stream depth and width is the same over the entire length of the segment.

Note 17: If the Lake (LAK3) Package (Merritt and Konikow, 2000) is also implemented, then flow out of the lake into a stream segment is dependent on the option used to compute stream depth (ICALC = 1, 2, 3, or 4). Constant discharge from a lake can be simulated no matter what value of ICALC is assigned to the stream segment emanating from the lake by assigning a positive value to FLOW in Part 4b.

Note 18: If a diversionary flow is large enough to warrant representation in the model, but is discharged into a pipeline, lined canal, or other structure or system that does not interact with the aquifer and the flow might exceed the available streamflow, then there is an alternative means to represent it. Instead of specifying a negative value of FLOW, we suggest representing the withdrawal by a single-reach diversionary stream segment, which would be

located in the same model cell as the reach from the upstream segment (IUPSEG) from which the diversion is made; specifying the segment's streambed hydraulic conductivity equal to 0 will preclude interaction with the aquifer and setting OUTSEG = 0 will remove the flow from the system. The diversion will then be subject to the constraints associated with the value of IPRIOR.

FOR EACH STRESS PERIOD:

5. Data: ITMP IRDFLG IPTFLG {NP}

ITMP — An integer value for reusing or reading stream segment data that can change each stress period. ITMP = 0 when all stream segment data is defined by Item 4 (NSFRPAR > 0; number of stream parameters is greater than 0). If ITMP < 0, then stream segment data not defined in Item 4 will be reused from the last stress period (Item 6 is not read for the current stress period). If ITMP > 0, then stream segment data not defined in Item 4 (for a number of segments equal to the value of ITMP) will be defined in Item 6 below. ITMP must be defined ≥ 0 for the first stress period of a simulation.

IRDFLG — An integer value for printing input data specified for this stress period. If IRDFLG = 0, input data for this stress period will be printed. If IRDFLG > 0, then input data for this stress period will not be printed.

IPTFLG — An integer value for printing streamflow-routing results during this stress period. If IPTFLG = 0, or whenever the variable ICBCFL is specified, the results for specified time steps during this stress period will be printed. If IPTFLG > 0, then the results during this stress period will not be printed.

NP — An integer value of the number of parameters used in the current stress period. The parameters being used are subsequently listed in Item 7 below. NP and Item 7 below are not read when NSFRPAR = 0.

Note 20: In each stress period, the sum of ITMP plus the sum of all NLST values in Item 3 associated with the NP parameters listed in Item 7 must equal or be less than (some stream segments may not be active during a stress period) the total number of stream segments in the stream network (NSS of Item 1). Stream segments defined by Items 3, 4, and 7 cannot be repeated using ITMP and Item 6.

Items 6a and 6b: Items 6a and 6b may include no input when all are defined by stream reaches in Item 2 or they may include as many as nine variables, depending on the values of REACHINPUT, ISFROPT, and ICALC specified in Items 1 and 4a.

If ITMP > 0:

6a. Data: NSEG ICALC OUTSEG IUPSEG {IPRIOR} {NSTRPTS} FLOW RUNOFF ETSW PPTSW {ROUGHCH} {ROUGHBK} {CDPTH} {FDPTH} {AWDTH} {BWDTH}

See Item 4, Part 4b for variable definitions in item 6a.

6b. Data: {HCOND1} {THICKM1} {ELEVUP} {WIDTH1} {DEPTH1} {THTS1} {THTI1} {EPS1} {UHC1}

HCOND1 Hydraulic conductivity of the streambed at the upstream end of this segment (units of length per time). This variable is read for each stress period when NSTRM is positive or when REACHINPUT has been specified and ISFROPT is 0, 4, or 5.

THICKM1 Thickness of streambed material at the upstream end of this segment (in units of length). This variable is read each stress period for all segments when NSTRM is positive or when REACHINPUT has been specified and ISFROPT is 0. When ISFROPT is 4 or 5, the variable is read each stress period for a segment when ICALC is 0, 3, or 4, and is read only the first stress period when ICALC is 1 or 2.

ELEVUP Elevation of the top of the streambed at the upstream end of this segment (in units of length). This variable is read each stress period for all segments when NSTRM is positive or when REACHINPUT has been specified and ISFROPT is 0. When ISFROPT is 4 or 5, the variable is read each stress period for a segment when ICALC is 0, 3, or 4, and is read only the first stress period when ICALC is 1 or 2.

WIDTH1 Average width of the stream channel at the upstream end of this segment (in units of length). This variable is read each stress period for all segments identified with an ICALC of 0 and is not dependent on ISFROPT. When ICALC is 1, the variable is read each stress period when NSTRM is positive or when REACHINPUT has been specified and ISFROPT is 0 or 1, and is read only for the first stress period when ISFROPT is 2, 3, 4, or 5.

DEPTH1 Average depth of water in the channel at the upstream end of this segment (units of length). This variable is only specified if ICALC is 0 and is not dependent on the value of NSTRM or ISFROPT. The stream stage in a reach is assumed to equal the elevation of the top of the streambed plus the depth of water.

THTS1 Saturated volumetric water content in the unsaturated zone beneath the upstream end of this segment. This variable is read for the first stress period when ICALC is 1 or 2 and ISFROPT is 4 or 5.

THTI1 Initial volumetric water content beneath the upstream end of this segment. THTI1 must be less than or equal to THTS and greater than or equal to THTS minus the specific yield defined in either LPF, BCF, or HUF. This variable is read for the first stress period when ICALC is 1 or 2 and ISFROPT is 4 or 5.

EPS1 Brooks-Corey exponent used in the relation between water content and hydraulic conductivity within the unsaturated zone beneath the upstream end of this segment. This variable is read for the first stress period when ICALC is 1 or 2 and ISFROPT is 4 or 5.

UHC1 Vertical saturated hydraulic conductivity of the unsaturated zone beneath the upstream end of this segment. This variable is necessary when using BCF or HUF, whereas it is optional when using LPF. This variable is read only for the first stress period when ICALC is 1 or 2 and ISFROPT is 5.

6c. Data: {HCOND2} {THICKM2} {ELEVDN} {WIDTH2} {DEPTH2}{THTS2} {THTI2} {EPS2} {UHC2}

HCOND2 Hydraulic conductivity of the streambed at the downstream end of this segment (units of length per time). This variable is read for each stress period when NSTRM is positive or when REACHINPUT has been specified and ISFROPT is 0, 4, or 5.

THICKM2 Thickness of streambed material at the downstream end of this segment (in units of length). This variable is read each stress period for all segments when NSTRM is positive or when REACHINPUT has been specified and ISFROPT is 0. When ISFROPT is 4 or 5, the variable is read each stress period for a

segment when ICALC is 0, 3, or 4, and is read only the first stress period when ICALC is 1 or 2.

ELEVDN Elevation of the top of the streambed at the downstream end of this segment (in units of length). This variable is read each stress period for all segments when NSTRM is positive or when REACHINPUT has been specified and ISFROPT is 0. When ISFROPT is 4 or 5, the variable is read each stress period for a segment when ICALC is 0, 3, or 4, and is read only the first stress period when ICALC is 1 or 2.

WIDTH2 Average width of the stream channel at the downstream end of this segment (in units of length). This variable is read each stress period for all segments identified with an ICALC of 0 and is not dependent on ISFROPT. When ICALC is 1, the variable is read each stress period when NSTRM is positive or when REACHINPUT has been specified and ISFROPT is 0 or 1, and is read only for the first stress period when ISFROPT is 2, 3, 4, or 5.

DEPTH2 Average depth of water in the channel at the downstream end of this segment (units of length). This variable is only specified if ICALC is 0 and is not dependent on the value of NSTRM or ISFROPT. The stream stage in a reach is assumed to equal the elevation of the top of the streambed plus the depth of water.

THTS2 Saturated volumetric water content in the unsaturated zone beneath the downstream end of this segment. This variable is read for the first stress period when ICALC is 1 or 2 and ISFROPT is 4 or 5.

THTI2 Initial volumetric water content beneath the downstream end of this segment. THTI2 must be less than or equal to THTS and greater than or equal to THTS minus the specific yield defined in either LPF, BCF, or HUF. This variable is read for the first stress period when ICALC is 1 or 2 and ISFROPT is 4 or 5.

EPS2 Brooks-Corey exponent used in the relation between water content and hydraulic conductivity within the unsaturated zone beneath the downstream end of this segment. This variable is read for the first stress period when ICALC is 1 or 2 and ISFROPT is 4 or 5.

UHC2 Vertical saturated hydraulic conductivity of the unsaturated zone beneath the downstream end of this segment. This variable is necessary when using BCF or HUF, whereas it is optional when using LPF. This variable is read only for the first stress period when ICALC is 1 or 2 and ISFROPT is 5.

Note 21: Stream properties and stresses are assumed to be constant and uniform within a single stream segment. Additionally, hydraulic conductivity, streambed thickness, elevation of the top of streambed, stream width, and stream depth may vary smoothly and linearly within a single stream segment. For these variables, data values at the upstream end of the segment are described in Item 4b and data values at the downstream end of the segment are described in Item 4c. Values of these variables for individual reaches of a segment are estimated using linear interpolation. To make any variable the same throughout the segment, simply specify equal values in Items 4b and 4c. The two elevations in Items 4b and 4c are used in conjunction with the total length of the stream segment (calculated from RCHLEN given for each reach in Item 2) to compute the slope of the stream and the elevations for any intermediate reaches. The streambed thickness is subtracted from the top of the streambed elevations to calculate the elevations of the bottom of the streambed (used in calculations of leakeage).

If ICALC = 2:

6d. Data: XCPT1 XCPT2 **...** XCPT8
Data: ZCPT1 ZCPT2 **...** ZCPT8

See Item 4, Part 4e for variable definitions. These variables are read only for the first stress period when ISFROPT is 2, 3, 4, or 5.

If ICALC = 4:

6e. Data: FLOWTAB(1) FLOWTAB(2) **...** FLOWTAB(NSTRPTS)
Data: DPTHTAB(1) DPTHTAB(2) **...** DPTHTAB(NSTRPTS)
Data: WDTHTAB(1) WDTHTAB(2) **...** WDTHTAB(NSTRPTS)

If keyword TABFILES has been specified, repeat Item 4f NUMTAB times for the first stress period only:

4f. Data: SEGNUM NUMVAL IUNIT

SEGNUM An integer value equal to the segment number to which the specified inflows will be applied.

NUMVAL An integer value equal to the number of rows in the tabular inflow file. Each inflow file may contain a different number of rows, but the number of rows in any file cannot exceed MAXVAL specified in Item 1b.

IUNIT An integer value equal to the unit number of the tabular inflow file. IUNIT must match the unit number for the file specified in the Name File.

Note 22: The external files that contain the specified inflows are referred to as tabular flow files. Each tabular file consists of two columns of input that are read using free format: TIME and INFLOW. Time is the point in the simulation when the inflow is specified for the segment; INFLOW is the specified flow, in units of length cubed per time. The units for TIME and INFLOW should be consistent with those specified for variables ITMUNI and LENUNI in the MODFLOW Discretization File. Times listed in the tabular flow file do not need to correspond to the beginning of MODFLOW time steps. If the beginning of the MODFLOW time steps fall between times listed in the tabular flow file, then the specified inflow is calculated using a time-weighted average of specified flows within the MODFLOW time step. Times can be listed in the tabular flow file either more frequently or less frequently than the MODFLOW time steps.

Note 23: Item 6 must be completed ITMP times. The data need not be defined in sequential order by stream segment number. All active segments in the stream network must be defined for each stress period through a combination of ITMP and Item 6 and NP and Item 7.

Note 24: If ITMP ≤ 0, then Item 6 is excluded for this stress period. If ITMP < 0, then values for Item 6 from the previous stress period are reused. If ITMP = 0, then no Item 6 records are read, and all segments must be defined using parameters.

Note 26: All the explanatory notes applicable to Item 4 (except those related to parameters) are also relevant to Item 6.

If NP > 0, then:

7. Data: Pname [Iname]

Pname The name of a parameter that is being used in the current stress period. Repeat Item 7 NP times (see Item 5).

Iname An instance name that is read only if Pname is a time-varying parameter. Multiple instances of the same time-varying parameter are not allowed in a stress period.

Example SFR2 input file demonstrating the use of the REACHINPUT and TABFILES functionalities

The following is part of an example SFR2 input file that demonstrates the REACHINPUT and TABFILES functionalities. The example was developed from the 'testsfr2' example that is provided with the MODFLOW-USG distribution. The example uses one stream segment that consists of 100 reaches:

```
# SFR2 Package input file for hypothetical test simulation
# Example using keyword options
REACHINPUT Item 1a
TABFILES 1 50 Item 1b
100 1 0 0 1.0 0.00001 -1 0 5 10 5 20 0 Item 1c: NSTRM NSS NSFRPAR
NPARSEG CONST DLEAK ISTCB1 ISTCB2 {ISFROPT} {NSTRAIL} {ISUZN}
{NSFRSETS} {IRTFLG}
1 4 1 1 1 200.0                          Item 2
1 4 2 1 2 200.0
1 4 3 1 3 200.0
      … (97 lines of input deleted here)
1 0 0 0                                  Item 3: stress period 1
1 2 0 0 .3 0.0 0.0 0.0 0.030 .04         Item 4a:
.00000035 0.5 140. .3 .1 3.5 6.0e-6      Item 4b:
.00000035 0.5 110. .3 .1 3.5 6.0e-6      Item 4c:
0. 2. 4. 6. 8. 10. 12. 14.               Item 4d:
6.0 4.5 3.5 0. 0.3 3.5 4.5 6.            Item 4d:
1 50 55                                  Item 4f: SEGNUM NUMVAL IUNIT
```

The tabular flow file has been assigned IUNIT 55 and Fname 'testsfr2.tab' in the Name File:

```
data 55 testsfr2.tab
```

File 'testsfr2.tab' has 50 lines of data, the first five of which are:

```
0 0.30                TIME INFLOW
2592000 2.53
5184000 3.84
7776000 17.85
10368000 20.26
```

The time and inflow values specified in each tabular flow file are echoed to the MODFLOW-USG LIST file.

LAKE (LAK7) PACKAGE INPUT INSTRUCTIONS – WITH SOLUTE TRANSPORT

Input Instructions

Solute transport capability was added to the LAK package of USG-T. This documentation was specifically created to outline the solute transport input that is needed for the LAK package. The input structure for LAK package solute transport follows the input requirements of MOC3D solute transport for the LAK package. Input instructions for the lake (LAK) package documented here are primarily reproduced from Merritt and Konikow (2000).

MODFLOW Name File

The simulation of the interaction of lakes with the aquifer is activated by including a record in the MOD- FLOW name file using the file type (Ftype) “LAK” to indicate that such calculations are to be made in the model and to specify the related input data file. The user can optionally specify that lake stages are to be written using the Gage Package by including a record in the MODFLOW name file using the file type (Ftype) “GAGE” that specifies the selected input data file identifying the lakes.

Lake Package Input Data

Input for the Lake Package is read from the unit specified in the MODFLOW name file. The input consists of nine separate data sets, each consisting of one or more records, as described in detail below. These data are used to specify information about the physical geometry of the lakes, hydraulic properties of the lakebeds, and the degree of hydraulic stress originating from atmospheric and anthropogenic sources, as well as specifying certain output control parameters. Spatial and temporal units of input data specifications should be consistent with other data input for the MODFLOW run.

In the following section, parameters are indicated as being optional by their enclosure in brackets. All input variables are read using free formats, unless specifically indicated otherwise. In free format, variables are separated by one or more spaces, or by a comma and, optionally, one or more spaces. It is important to note that, in free format, blank spaces are not read as zeroes and a blank field cannot be used to set a parameter value to zero. The input instructions below are reproduced from Merritt and Konikow (2000) for the solute transport aspect of LAK package, however, these input instructions are specifically listed to work with the transport

version of MODFOW-USG. Any new additions or changes specifically made for USG-T are highlighted with blue colored text.

FOR EACH SIMULATION

Record 1b. Data: {TABLEINPUT} {TRANSPORTBOUNDARY}

TABLEINPUT–An optional character variable used for activating the option to specify text files containing relations among lake stage, surface area, and volume. A separate text file is specified for each lake; each file contains exactly 151 lines; and each line consists of one value for lake stage, volume, and surface area, respectively. This file must contain exactly 151 lines of data because this number of values is consistent with the number of values that are calculated internally by the Lake Package if the "TABLEINPUT" option is not used and ensures that results will be consistent with results for simulations that calculate lake bathymetry information internally. For example, Lake Package test problems can be run without using the "TABLEINPUT" option and the Lake Package will output the lake bathymetry tables as 151 values to the List file. Bathymetry values printed to the List file can then be used directly for specifying a separate bathymetry input file using the keyword option "TABLEINPUT" and the solution will be the same. However, for difficult problems convergence can be improved by smoothing the lake bathymetry data (for example, by fitting polynomial regression equations to the original bathymetry information). If the keyword "TABLEINPUT" is entered on the first line (record) of the data set, then lake bathymetry data will be read from separate input files. These tables are used for calculating water balances within lakes; however, calculation of seepage between lakes and groundwater is unchanged from the original Lake Package on the basis of the lake and groundwater discretization (Merritt and Konikow, 2000). See IUNITTAB.

TRANSPORTBOUNDARY–For solute transport simulations this keyword enables simulating lakes only as a boundary condition. When this keyword is activated, solute transport within lakes will not be simulated and lakes will be treated only as a boundary condition to the groundwater system enabling solute flux in and out of lakes. With this keyword, the only solute transport input needed in the LAK package is CLAKBC as listed below. Other solute transport input (CLAKE, CPPT, CRNF, CAUG) is not required with this keyword. If solute transport is not simulated, this keyword is not required, and if entered, will be ignored.

Record 1b. Data: NLAKES ILKCB

NLAKES–Number of separate lakes.

ILKCB–Whether or not to write cell-by-cell flows (yes if ILKCB> 0, no otherwise). If ILKCB< 0 and ICBCFL is not equal to 0, the cell-by-cell flows will be printed in the standard output file.

Notes:

1. Sublakes of multiple-lake systems are considered separate lakes for input purposes. The variable NLAKES is used, with certain internal assumptions and approximations, to dimension arrays for the simulation.
2. If data are being read using the fixed format mode, then each field should be entered using I10 format.
3. ICBCFL is specified in the input to the Output Control Package of MODFLOW.

Record 2. Data: THETA {NSSITR SSCNCR}

THETA–Explicit (THETA = 0.0), semi-implicit (0.0 < THETA < 1.0), or implicit (THETA = 1.0) solution for lake stages.

NSSITR–Maximum number of iterations for Newton's method solution for equilibrium lake stages in each MODFLOW iteration for steady-state aquifer head solution. Only read if ISS (option flag input to BCF Package of MODFLOW indicating steady-state solution) is not zero.

SSCNCR–Convergence criterion for equilibrium lake stage solution by Newton's method. Only read if ISS is not zero.

Notes:

1. NSSITR and SSCNCR are not needed for a transient solution (ISS = 0) and should be omitted when the solution is transient.
2. If data are being read using the fixed format mode, then the data should be entered using format (F10.4, I10, F10.4).

3. THETA should be set equal to zero if a steady-state solution is to be performed.

For the First Stress Period Only:

Record 3. Data: STAGES {SSMN SSMX} {CLAKE(1). CLAKE(NSOL)}

STAGES–The initial stage of each lake at the beginning of the run.

SSMN–Minimum stage allowed for each lake in steady-state solution.

SSMX–Maximum stage allowed for each lake in steady-state solution.

CLAKE–The initial concentrations in each lake at the beginning of the model run. Values are entered for NSOL constituents. The value of NSOL is passed from USG-T. CLAKE values are ignored if entered in MODFLOW runs. If keyword TRANSPORTBOUNDARY is activated, CLAKE is neither required nor used.

Notes:

1. This data set should consist of one line for each lake, where line 1 includes data for lake 1, and line n includes data for lake n. There must be exactly NLAKES lines of data.
2. SSMN and SSMX are not needed for a transient run and must be omitted when the solution is transient.
3. CLAKE is an optional parameter, and is only read if solute transport is being simulated. In that case, if more than one solute is being simulated, then there should be a string of NSOL values of CLAKE (where NSOL is the number of solutes) on one line. The default value of NSOL is NSOL = 1.
4. If data are being read using the fixed format mode, then each field should be entered using F10.4 format.

For Each Stress Period:

Record 4. Data: ITMP ITMP1 LWRT

ITMP–> 0, read lake definition data (records 5-7, and, optionally, records 8 and 9);

= 0, no lake calculations this stress period;

< 0, use lake definition data from last stress period.

ITMP1–> 0 or = 0, read new recharge, evaporation, runoff, and withdrawal data for each lake, and associated concentrations if needed for USG-T runs;

< 0, use recharge, evaporation, runoff, and withdrawal data, and concentrations, if needed, from last stress period.

LWRT–> 0, suppresses printout from the lake package.

Notes:

1. ICBCFL < 0 or = 0 also suppresses printout from the lake package. ICBCFL is specified in the input to the Output Control Package of MODFLOW.
2. If data are being read using the fixed format mode, then each field should be entered using I10 format.
3. Lake definition data are restricted to cells for which IBOUND and WETDRY values have been set to zero.

If ITMP > 0:

Record 5. Data: LKARR(NCOL,NROW)

A NCOL by NROW array is read for each layer in the grid by MODFLOW module U2DINT.

LKARR–A value is read in for every grid cell. If LKARR(I,J,K) = 0, the grid cell is not a lake volume cell.

If LKARR(I,J,K) > 0, its value is the identification number of the lake occupying the grid cell. LKARR(I,J,K) must not exceed the value NLAKES. If it does, or if LKARR(I,J,K) < 0,

LKARR(I,J,K) is set to zero.

Notes:

1. Lake cells cannot be overlain by non-lake cells in a higher layer.

Record 6. Data: BDLKNC(NCOL,NROW)

A NCOL by NROW array is read for each layer in the grid by MODFLOW module U2DREL.

BDLKNC–A value is read in for every grid cell. The value is the lakebed leakance that will be assigned to lake/aquifer interfaces that occur in the corresponding grid cell.

Notes:

1. If the wet-dry option flag (IWTFLG) is not active (cells cannot rewet if they become dry), then the BDLKNC values are assumed to represent the combined leakances of the lakebed material and the aquifer material between the lake and the centers of the underlying grid cells, i.e., the vertical conductance values (CV) will not be used in the computation of conductances across lake/aquifer boundary faces in the vertical direction.
2. IBOUND in the input to the Basic Package of MODFLOW and, if the IWTFLG option is active, WETDRY in the input to the BCF or other flow package of MODFLOW, should be set to zero for every cell for which LKARR is not equal to zero.

If ITMP > 0:

Record 7. Data: NSLMS

NSLMS–The number of sublake systems if coalescing/dividing lakes are to be simulated (only in transient runs). Enter 0 if no sublake systems are to be simulated.

Notes:

1. If data are being read using the fixed format mode, then NSLMS should be entered using format I5.

If ITMP > 0 and NSLMS > 0:

Record 8a. Data: IC ISUB(1) ISUB(2) ISUB(IC)

Record 8b. Data: SILLVT(2) SILLVT(IC)

IC–The number of sublakes, including the center lake, in the sublake system being described in this record.

ISUB–The identification numbers of the sublakes in the sublake system being described in this record. The center lake number is listed first.

SILLVT–Sill elevation that determines whether the center lake is connected with a given sublake. One value is entered in this record for each sublake in the order the sublakes are listed in the previous record.

Notes:

1. A pair of records (records 8a and 8b) is read for each multiple-lake system, i.e., NSLMS pairs of records. However, IC = 0 will terminate the input.
2. If data are being read using the fixed format mode, then each field of Record 8a should be entered using I5 format and each field of Record 8b should be entered using F10.4 format.

If ITMP1 > 0 or = 0.

Record 9a. Data: PRCPLK EVAPLK RNF WTHDRW

PRCPLK–The rate of precipitation per unit area at the surface of a lake (L/T).

EVAPLK–The rate of evaporation per unit area from the surface of a lake (L/T).

RNF–Overland runoff from an adjacent watershed entering the lake. If RNF > 0, it is specified directly as volumetric rate, or flux (L3/T). If RNF < 0, its absolute value is used as a dimensionless multiplier applied to the product of the lake precipitation rate per unit area (PRCPLK) and the surface area of the lake at its full stage (occupying all layer 1 lake cells).

WTHDRW–The volumetric rate, or flux (L3/T), of water removal from a lake by means other than rainfall, evaporation, surface outflow, or ground-water seepage. A negative value indicates augmentation. Normally, this would be used to specify the rate of artificial withdrawal from a lake for human water use, or if negative, artificial augmentation of a lake volume for esthetic or recreational purposes.

Notes:

1. When RNF is entered as a dimensionless multiplier (RNF < 0), it is considered to be the product of two proportionality factors. The first is the ratio of the area of the basin

contributing runoff to the surface area of the lake when it is at full stage. The second is the fraction of the current rainfall rate that becomes runoff to the lake. This procedure provides a means for the automated computation of runoff rate from a watershed to a lake as a function of varying rainfall rate. For example, if the basin area is 10 times greater than the surface area of the lake, and 20 percent of the precipitation on the basin becomes overland runoff directly into the lake, then set RNF = -2.0.

If solute transport is also being simulated, then for each solute the following data are read. If keyword TRANSPORTBOUNDARY is activated then Record 9b is ignored and Record 9c is read.

Record 9b. Data: CPPT(NSOL) CRNF(NSOL) {CAUG(NSOL)}

CPPT–The concentration of solute in precipitation onto the lake surface.

CRNF–The concentration of solute in overland runoff directly into the lake.

CAUG–The concentration of solute in water used to augment the lake volume.

Notes:

1. At least one of the above records will be read for each lake; i.e., NLAKES records, or sets of records, will be read. If MODFLOW is being run, only the first record is read. If USG-T is being run, a set of two or more records will be read for each lake (see note 2).
2. If record 9b is included because solute transport is being simulated, then 9b should consist of one record (line) for each solute; each record must contain two or three values; and there must be as many records as the number of solutes being simulated (NSOL). The order of records must be that all necessary lines for 9b are listed for a given lake before line 9a for the next lake. For example, if the Lake Package is representing three lakes and the solute transport package is representing two solutes, then the order of data for Record 9 would be 9a, 9b, 9b, 9a, 9b, 9b, 9a, 9b, and 9b.
3. CAUG is an optional parameter and is only read if the value of WTHDRW in 9a is negative (no value should be specified for CAUG if WTHDRW in 9a is positive, indicating withdrawal of water from the lake).

4. It is implicitly assumed that no solute is present in water evaporated from the lake surface.
5. If data are being read using the fixed format mode, then each field should be entered using F10.4 format.

Record 9c is read only if solute transport is being simulated and if keyword TRANSPORTBOUNDARY is active.

Record 9c. Data: CLAKBC(NSOL)

CLAKBC–The concentration of solute for lake boundary. CLAKBC is the concentration that will be used to calculate solute influx from lake boundary into the groundwater system when lakes are treated as a boundary condition to the groundwater system.

GAGE (GAGE) PACKAGE FOR MONITORING STATION INPUT INSTRUCTIONS

Lakes can be designated as having gaging stations located on them. For each such designated lake, the time and stage of that lake (and if solute transport is being simulated, the concentration of each solute) after each time step (and each transport time increment) will be written to a separate output file to facilitate graphical post-processing of the calculated data. The input file for specifying gaging station locations is read if the file type (Ftype) "GAGE" is included in the MODFLOW name file.

For each simulation, if GAGE Package is used:

Record 1: Data: NUMGAGE

NUMGAGE Number of gaging stations

For each gaging station:

Record 2: Data: LAKE UNIT {OUTTYPE}

LAKE–Negative value of the lake number of the lake where the gage is located.

UNIT –Unit number for output file.

OUTTYPE–OUTTYPE Code for type of expanded listing desired in output file:

0. Use standard default listing of time, stage, volume, and concentration.

1. Default values plus all inflows to and outflows from lake (as volumes during time increment), total lake conductance, and time-step budget error (percent). Computed runoff from UZF and lake infiltration to UZF is added whenever the UZF Package is active in MODFLOW-2005 and MODFLOW-LGR. (The UZF Package is not available in MODFLOW-2000.)

2. Default values plus changes in lake stage, lake volume, and solute concentrations, and cumulative lake budget error (percent).

3. All of the above except time-step budget error.

4. Time, lake stage, lake volume, solute concentration, and rate of change of lake volume, as well as volumetric rates for all inflows to and outflows from lakes (L3/T), total lake conductance (L2/T), and time-step budget error. Volumetric rates of computed runoff from UZF and lake infiltration to UZF is added whenever the UZF Package is active in MODFLOW-2005, MODFLOW-CFP, MODFLOW-NWT, and MODFLOW-LGR.

Total lake conductance (OUTTYPE options 1 and 3 for a lake gaging station) is the sum of the conductances of each seepage interface for each lake. Changes in lake stage, volume, and solute concentrations (OUTTYPE options 2 or 3) are listed as incremental changes from previous time increment and as cumulative change since start of simulation. Volumetric rates for option 4 are expressed in units of volume per time during a time step increment. Versions of the GAGE Package since 2006 for MODFLOW-2000 and MODFLOW-2005 had listed groundwater inflows and outflows as volumetric flow rates and listed the other values as volumes per time step for options 1 and 3. Versions of the GAGE Package since 2006 for MODFLOW-2000 and MODFLOW-2005 had listed groundwater inflows and outflows as volumetric flow rates and listed the other values as volumes per time step for options 1 and 3.

Notes:

1. The user should specify a unique unit number for each gaging station and match those unit numbers to DATA file types and file names in the MODFLOW name file (Harbaugh and McDonald, 1996b).

2. The Gage Package can also be used in conjunction with the Stream Package to specify the location of a gaging station on a stream. Therefore, to guarantee that the code can distinguish between input for lakes and that for stream locations, lake numbers are specified as their negative value.

Data Set 2 must include exactly NUMGAGE lines (or records) of data. If NUMGAGE > 1, it is permissible to interleaf in Data Set 2 records for stream gaging stations (according to the format specified in the documentation for the Stream Package) with records for gages on lakes (according to the format described above). Data lines (records) within Data Set 2 can be listed in any arbitrary order.

SPECIFIED GRADIENT BOUNDARY (SGB) PACKAGE INPUT INSTRUCTIONS

Input for the Specified Gradient Boundary (SGB) Package is read from the file that has file type "SGB" in the Name File. All variables are read in free format if the option "FREE" is specified in the Basic Package input file; otherwise, the non-optional variables have 10-character fields and the optional variables are free format.

Note that the SGB package applies to all process domains including the GWF and CLN Processes. Note that this input is read only in an unstructured format, even if the structured format option is selected. However, output of cell-by-cell fluxes will be in a structured format, if the structured option is used for the model.

The SGB package does not support solute or heat transport. **Thus, if a solute reaches a SGB boundary, it will accumulate at the boundary and will not be let out with the water.**

FOR EACH SIMULATION

0. [#Text]

   Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1a. [***PARAMETER*** NPSGB MXL]

   This optional item must start with the word "PARAMETER".

2. MXSGB ISGBCB

3. [PARNAM PARTYP Parval NLST [***INSTANCES*** NUMINST]]

   Repeat Item 3 combined with the indicated repetitions of Item 4 NPSGB times. Items 3 and 4 are not read if NPSGB is negative or 0.

   If PARNAM is to be a time-varying parameter, the keyword "INSTANCES" and a value for NUMINST must be entered.

4a. [INSTNAM]

4b. Node SGfact [xyz]

   After each Item 3 for which the keyword "INSTANCES" is not entered, read Item 4b, and not Item 4a.

   After each Item 3 for which the keyword "INSTANCES" is entered, read Item 4a and Item 4b for each instance.

   NLST repetitions of Item 4b are required; they are read by subroutine ULSTRD. (SFAC of the ULSTRD utility subroutine applies to Qfact). The NLST repetitions of Item 4b follow each repetition of Item 4a when PARNAM is time varying.

FOR EACH STRESS PERIOD

5. ITMP NP

6a. Node SG [xyz]

   (ITMP repetitions of Item 6a are read by subroutine ULSTRD if ITMP > 0. (SFAC of the ULSTRD utility subroutine applies to Q.) Item 6a is not read if ITMP is negative or zero.

7. [Pname [Iname]]

   (Item 7 is repeated NP times. It is not read if NP is negative or 0. Iname is read if Pname is a time-varying parameter.)

Explanation of Variables Read by the SGB Package:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPSGB—is the number of specified gradient boundary parameters.

MXL—is the maximum number of SGB cells that will be defined using parameters.

MXSGB—is the maximum number of SGB cells in use during any stress period, including those that are defined using parameters.

ISGBCB—is a flag and a unit number.

If ISGBCB > 0,	cell-by-cell flow terms will be written to this unit number when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control.
If ISGBCB = 0,	cell-by-cell flow terms will not be written.
If ISGBCB < 0, S	GB cell flux for each cell will be written to the listing file when "SAVE BUDGET" or a nonzero value for ICBCFL is specified in Output Control.

Option—is an optional list of character values.

"AUXILIARY abc" or "AUX abc"—defines an auxiliary variable, named "abc", which will be read for each SGB cell as part of Items 4 and 6. Up to 20 variables can be specified, each of which must be preceded by "AUXILIARY" or "AUX." These variables will not be used by the Ground-Water Flow Process, but they will be available for use by other processes. The auxiliary variable values will be read after the Q variable.

"NOPRINT"—specifies that lists of SGB cells will not be written to the Listing File.

PARNAM—is the name of a parameter. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter. For the SGB Package, the only allowed parameter type is SG, which defines values of the specified gradient.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NLST—is the number of SGB cells in a non-time-varying parameter. For a time-varying parameter, NLST is the number of SGB cells in each instance.

INSTANCES—is an optional keyword that designates a parameter as time varying. The keyword is not case sensitive; that is, any combination of the same characters with different case can be used. If ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, PARNAM is non-time-varying and NUMINST should not be present.

NUMINST—is the number of instances for a time-varying parameter, where each instance is a list of river reaches and associated properties. If the keyword ***INSTANCES*** is present, it must be followed by a value for NUMINST. If ***INSTANCES*** is absent, NUMINST should not be present.

INSTNAM—is the name of an instance associated with the parameter named in the corresponding Item 3. The instance name can be 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent. Instance names must be unique for a parameter, but instance names may be reused for different parameters.

Node—is the global node number of the model cell (GWF cell or CLN cell) that contains the SGB cell. The global node number of a GWF cell for a structured grid may be computed as (KLAY-1)*NROW*NCOL + (IROW-1)*NCOL + JCOL where KLAY is the layer number, IROW is the row number and JCOL is the column number of the GWF Process cell. For a CLN cell, the global node number is the CLN cell node number plus the total number of GWF Process cells.

SGfact—is the factor used to calculate SGB cell flux rate from the parameter value. The flow rate is the product of SGfact and the parameter value.

[xyz]—represents the values of the auxiliary variables for a SGB cell that have been defined in Item 2. The values of auxiliary variables must be present in each repetition of Items 4 and 6 if they are defined in Item 2. The values must be specified in the order used to define the variables in Item 2.

ITMP—is a flag and a counter for subsurface nodes.

If ITMP < 0, non-parameter SGB cell data from the last stress period for subsurface nodes will be reused.

ITMP ≥ 0, ITMP will be the number of non-parameter SGB cells read for the current stress period for subsurface nodes.

NP—is the number of parameters in use in the current stress period.

SG—is the specified gradient. A positive value indicates inflow and a negative value indicates outflow. The gradient times flow area times the anisotropy ratio is entered here.

Pname—is the name of a parameter that is being used in the current stress period. NP parameter names will be read.

Iname—is an instance name that is read only if Pname is a time-varying parameter. Multiple instances of the same parameter are not allowed in a stress period.

SUBSIDENCE (SUB) PACKAGE INPUT INSTRUCTIONS

Input for the SUB Package is read from the file that has the type "SUB" in the name file. Optional variables are shown in brackets. All single-valued variables in data items 1, 15, and 16, layer assignments for systems of interbeds in data items 2 and 3, and material properties in data item 9 are read in free format. Data items 1, 2, 3, and 15 consist of at most one record. For structured grids, the two-dimensional arrays in data items 4-8 and 10-14 are read with MODFLOW-2000 utility array readers U2DREL and U2DINT. For instructions on use of array readers, refer to Harbaugh and others (2000). For unstructured grids, the one-dimensional arrays in data items 4-8 and 10-14 are read with MODFLOW-USG utility array readers U1DREL and U1DINT.

FOR EACH SIMULATION

1. ISUBCB ISUBOC NNDB NDB NMZ NN AC1 AC2 ITMIN IDSAVE IDREST

(Enter integers for variables other than AC1 and AC2, which are floating-point variables.)

2. [LN(NNDB)] if NNDB > 0

(Enter NNDB integers separated by one or more spaces or by commas.)

3. [LDN(NDB)] if NDB > 0

(Enter NDB integers separated by one or more spaces or by commas.)

If *UNSTRUCTURED* option is used then read item 4a, or for structured grid read item 4b.

4a. [RNB(NODLAY(1))] U1DREL if NDB > 0, where NODLAY(1) is the number of nodes in layer 1.

4b. [RNB(NCOL,NROW)] U2DREL if NDB > 0

(One array for each of the NDB systems of interbeds)

The following four arrays are needed to describe the initial conditions and properties of each of the NNDB systems of no-delay interbeds. All of the arrays (items 5–8) for system 1 are read first; then all of the arrays for the remaining systems.

If *UNSTRUCTURED* option is used then read item 5a, or for structured grid read item 5b.

5a. [HC(NODLAY(1))] U1DREL if NNDB > 0, where NODLAY(1) is the number of nodes in layer 1.

5b. [HC(NCOL,NROW)] U2DREL if NNDB > 0

If *UNSTRUCTURED* option is used then read item 6a, or for structured grid read item 6b.

6a. [Sfe(NODLAY(1))] U1DREL if NNDB > 0, where NODLAY(1) is the number of nodes in layer 1.

6b. [Sfe(NCOL,NROW)] U2DREL if NNDB > 0

If *UNSTRUCTURED* option is used then read item 7a, or for structured grid read item 7b.

7a. [Sfv(NODLAY(1))] U1DREL if NNDB > 0, where NODLAY(1) is the number of nodes in layer 1.

7b. [Sfv(NCOL,NROW)] U2DREL if NNDB > 0

If *UNSTRUCTURED* option is used then read item 8a, or for structured grid read item 8b.

8a. [Com(NODLAY(1))] U1DREL if NNDB > 0, where NODLAY(1) is the number of nodes in layer 1.

8b. [Com(NCOL,NROW)] U2DREL if NNDB > 0

9. [DP(NMZ,3)] if NDB > 0

(Use one record for each material zone. Data item includes NMZ records, each with a value of vertical hydraulic conductivity, elastic specific storage, and inelastic specific storage)

The following five arrays are needed to describe the initial conditions and properties of each of the NDB systems of delay interbeds. All of the arrays (items 10-14) for system 1 are read first; then all of the arrays for the remaining systems.

If *UNSTRUCTURED* option is used then read item 10a, or for structured grid read item 10b.

10a. [Dstart(NODLAY(1))] U1DREL if NDB > 0, where NODLAY(1) is the number of nodes in layer 1.

10b. [Dstart(NCOL,NROW)] U2DREL if NDB > 0

If *UNSTRUCTURED* option is used then read item 11a, or for structured grid read item 11b.

11a. [DHC(NODLAY(1))] U1DREL if NDB > 0, where NODLAY(1) is the number of nodes in layer 1.

11b. [DHC(NCOL,NROW)] U2DREL if NDB > 0

If *UNSTRUCTURED* option is used then read item 12a, or for structured grid read item 12b.

12a. [DCOM(NODLAY(1))] U1DREL if NDB > 0, where NODLAY(1) is the number of nodes in layer 1.

12b. [DCOM(NCOL,NROW)] U2DREL if NDB > 0

If *UNSTRUCTURED* option is used then read item 13a, or for structured grid read item 13b.

13a. [DZ(NODLAY(1))] U1DREL if NDB > 0, where NODLAY(1) is the number of nodes in layer 1.

13b. [DZ(NCOL,NROW)] U2DREL if NDB > 0

If *UNSTRUCTURED* option is used then read item 14a, or for structured grid read item 14b.

14a. [NZ(NODLAY(1))] U1DINT if NDB > 0, where NODLAY(1) is the number of nodes in model layer 1.

14b. [NZ(NCOL,NROW)] U2DINT if NDB > 0

15. [Ifm1 Iun1 Ifm2 Iun2 Ifm3 Iun3 Ifm4 Iun4 Ifm5 Iun5 Ifm6 Iun6] if ISUBOC > 0

(Data item 15 consists of one record with 12 integers separated by one or more spaces or by commas)

16. [ISP1 ISP2 ITS1 ITS2 Ifl1 Ifl2 Ifl3 Ifl4 Ifl5 Ifl6 Ifl7 Ifl8 Ifl9 Ifl10 Ifl11 Ifl12 Ifl13] if ISUBOC > 0.

Data item 16 consists of ISUBOC records with 17 integers separated by one or more spaces or by commas. Please see the section entitled "Package Output" for a detailed explanation of the use of data item 16.

Explanation of Variables Read by the SUB Package:

ISUBCB is a flag and unit number.
- If ISUBCB > 0, it is the unit number to which cell-by-cell flow terms will be written when "SAVE BUDGET" or a non-zero value for ICBCFL is specified in MODFLOW-2000 Output Control (see Harbaugh and others, 2000, p. 52–55).
- If ISUBCB ≤ 0, cell-by-cell flow terms will not be recorded.

ISUBOC is a flag used to control output of information generated by the Sub Package
- If ISUBOC > 0, it is the number of repetitions of item 16 to be read, each repetition of which defines a set of times steps and associated flags for printing and saving subsidence, compaction, vertical displacement, preconsolidation head and volumetric budget.
- If ISUBOC ≤ 0, volumetric budgets for systems of delay interbeds will be printed at the end of each stress period. Subsidence, compaction, vertical displacement, preconsolidation head will not be printed or saved.

NNDB is the number of systems of no-delay interbeds.

NDB is the number of systems of delay interbeds.

NMZ is the number of material zones that are needed to define the hydraulic properties of systems of delay interbeds. Each material zone is defined by a

combination of vertical hydraulic conductivity, elastic specific storage, and inelastic specific storage.

NN is the number of nodes used to discretize the half space to approximate the head distributions in systems of delay interbeds.

AC1 is an acceleration parameter.This parameter (ω1 in equation 25) is used to predict the aquifer head at the interbed boundaries on the basis of the head change computed for the previous iteration. A value of 0.0 results in the use of the aquifer head at the previous iteration. Limited experience indicates that optimum values may range from 0.0 to 0.6.

AC2 is an acceleration parameter. This acceleration parameter is a multiplier for the head changes to compute the head at the new iteration (ω2 in equation 27). Values are normally between 1.0 and 2.0, but the optimum is probably closer to 1.0 than to 2.0. However, as discussed following equation 27, this parameter also can be used to help convergence of the iterative solution by using values between 0 and 1.

ITMIN is the minimum number of iterations for which one-dimensional equations will be solved for flow in interbeds when the Strongly Implicit Procedure (SIP) is used to solve the ground-water flow equations. If the current iteration level is greater than ITMIN and the SIP convergence criterion for head closure (HCLOSE) is met at a particular cell, the one-dimensional equations for that cell will not be solved. The previous solution will be used. The value of ITMIN is not used if a solver other than SIP is used to solve the ground-water flow equations.

IDSAVE is a flag and a unit number.

If IDSAVE > 0, it is the unit number on which restart records for delay interbeds will be saved at the end of the simulation. The unit number must be associated with a BINARY data file specified in the MODFLOW Name File.

If IDSAVE ≤ 0, restart records for delay interbeds will not be saved.

IDREST is a flag and a unit number.

If IDREST > 0, it is the unit number on which restart records for delay interbeds will be read in at the start of the simulation. The unit number must be associated with a BINARY data file specified in the MODFLOW Name File.

If IDREST ≤ 0, restart records for delay interbeds will not be read in.

LN is a one-dimensional array specifying the model layer assignments for each system of no-delay interbeds. The array has NNDB values.

LDN is a one-dimensional array specifying the model layer assignments for each system of delay interbeds. The array has NDB values.

RNB is an array specifying the factor *nequiv* (equation 20) at each cell for each system of delay interbeds. The array also is used to define the areal extent of each system of interbeds. For cells beyond the areal extent of the system of interbeds, enter a number less than 1.0 in the corresponding element of this array.

HC is an array specifying the preconsolidation head or preconsolidation stress in terms of head in the aquifer for systems of no-delay interbeds. For any model cells in which specified HC is greater than the corresponding value of starting head, the value of HC will be set to that of starting head.

Sfe is an array specifying the dimensionless elastic skeletal storage coefficient for systems of no-delay interbeds. Values may be estimated using equation 17.

Sfv is an array specifying the dimensionless inelastic skeletal storage coefficient for systems of no-delay interbeds. Values may be estimated using equation 17.

COM is an array specifying the starting compaction in each system of no-delay interbeds. Compaction values computed by the package are added to values in this array so that printed or stored values of compaction and land subsidence may include previous components. Values in this array do not affect calculations of storage changes or resulting compaction. For simulations in which output values are to reflect compaction and subsidence since the start of the simulation, enter zero values for all elements of this array.

DP is an array containing a table of material properties for systems of delay interbeds. For each of the NMZ zones of material properties, vertical hydraulic conductivity, elastic specific storage, and inelastic specific storage are read.

Dstart is an array specifying starting head in interbeds for systems of delay interbeds. For a particular location in a system of interbeds, the starting head is applied to every node in the string of nodes that approximates flow in half of a doubly draining interbed.

DHC is an array specifying the starting preconsolidation head in interbeds for systems of delay interbeds. For a particular location in a system of interbeds, the starting preconsolidation head is applied to every node in the string of nodes that approximates flow in half of a doubly draining interbed. For any location at which specified starting preconsolidation head is greater than the corresponding value of the starting head, Dstart, the value of the starting preconsolidation head will be set to that of the starting head.

DCOM is an array specifying the starting compaction in each system of delay interbeds. Compaction values computed by the package are added to values in this array so that printed or stored values of compaction and land subsidence may include previous components. Values in this array do not affect calculations of storage changes or resulting compaction. For simulations in which output values are to reflect compaction and subsidence since the start of the simulation, enter zero values for all elements of this array.

DZ is an array specifying the equivalent thickness for a system of delay interbeds (*b*equiv in equation 19).

NZ is an array specifying the material zone numbers for systems of delay interbeds. The zone number for each location in the model grid selects the hydraulic conductivity, elastic specific storage, and inelastic specific storage of the interbeds.

Ifm1 is a code for the format in which subsidence will be printed. Format codes for variables Ifm1, Ifm2, Ifm3, Ifm4, Ifm5, Ifm6 are as follows:

0 - (10G11.4)	7 - (20F5.0)
1 - (11G10.3)	8 - (20F5.1)

2 - (9G13.6)
3 - (15F7.1)
4 - (15F7.2)
5 - (15F7.3)
6 - (15F7.4)
9 - (20F5.2)
10 - (20F5.3)
11 - (20F5.4)
12 - (10G11.4)

Iun1 is the unit number to which subsidence will be written if it is saved on disk.

Ifm2 is a code for the format in which compaction by model layer will be printed.

Iun2 is the unit number to which compaction by model layer will be written if it is saved on disk.

Ifm3 is a code for the format in which compaction by interbed system will be printed.

Iun3 is the unit number to which compaction by interbed system will be written if it is saved on disk.

Ifm4 is a code for the format in which vertical displacement will be printed.

Iun4 is the unit number to which vertical displacement will be written if it is saved on disk.

Ifm5 is a code for the format in which no-delay preconsolidation head will be printed.

Iun5 is the unit number to which no-delay preconsolidation head will be written if it is saved on disk.

Ifm6 is a code for the format in which delay preconsolidation head will be printed.

Iun6 is the unit number to which delay preconsolidation head will be written if it is saved on disk.

The variables ISP1, ISP2, ITS1, ITS2, and Ifl1 through Ifl13 are used to control printing and saving of information generated by the SUB Package during program execution. The use of some of these variables is explained in more detail in the section entitled Package Output. The default condition for flags Ifl1 through Ifl13 is to not print or save the indicated information, except for printing budgets for no-delay interbeds for the last time step of each stress period.

ISP1 is the starting stress period in the range of stress periods to which output flags Ifl1 through Ifl13 apply. If the value of ISP1 is less than 1, the SUB Package will change the number to 1.

ISP2 is the ending stress period in the range of stress periods and time steps to which output flags Ifl1 through Ifl13 apply. If the value of ISP1 is greater than NPER (the number of stress periods in the simulation), the SUB Package will change the number to NPER.

ITS1 is the starting time step in the range of time steps in each of the stress periods ISP1 through ISP2 to which output flags Ifl1 through Ifl13 apply. If the value of ITS1is less than 1, the SUB Package will change the number to 1.

ITS2 is the ending time step in the range of time steps in each of stress periods ISP1 through ISP2 to which output flags Ifl1 through Ifl13 apply. If the value of ITS2 is greater than the number of time steps in a given stress period, the SUB Package will change the number to the number of time steps in that stress period.

Ifl1 is the output flag for printing subsidence for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl1 < 0, use default or previously defined settings of Ifl1 for printing subsidence.
If Ifl1 = 0, do not print subsidence.
If Ifl1 > 0, print subsidence.

Ifl2 is the output flag for saving subsidence to an unformatted disk file for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl2 < 0, use default or previously defined settings of Ifl2 for saving subsidence.
If Ifl2 = 0, do not save subsidence.
If Ifl2 > 0, save subsidence.

Ifl3 is the output flag for printing compaction by model layer for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl3 < 0, use default or previously defined settings of Ifl3 for printing compaction by model layer.
If Ifl3 = 0, do not print compaction by model layer.

If Ifl3 > 0, print compaction by model layer.

Ifl4 is the output flag for saving compaction by model layer to an unformatted disk file for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl4 < 0, use default or previously defined settings of Ifl4 for saving compaction by model layer.

If Ifl4 = 0, do not save compaction by model layer.

If Ifl4 > 0, save compaction by model layer.

Ifl5 is the output flag for compaction by interbed system printout for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl5 < 0, use default or previously defined settings of Ifl5 for printing compaction by interbed system.

If Ifl5 = 0, do not print compaction by interbed system.

If Ifl5 > 0, print compaction by interbed system.

Ifl6 is the output flag for saving compaction by interbed system to an unformatted disk file for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl6 < 0, use default or previously defined settings of Ifl6 for saving compaction by interbed system.

If Ifl6 = 0, do not save compaction by interbed system.

If Ifl6 > 0, save compaction by interbed system.

Ifl7 is the output flag for vertical displacement printout for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl7 < 0, use default or previously defined settings of Ifl7 for printing vertical displacement.

If Ifl7 = 0, do not print vertical displacement.

If Ifl7 > 0, print vertical displacement.

Ifl8 is the output flag for saving vertical displacement to an unformatted disk file for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl8 < 0, use default or previously defined settings of Ifl8 for saving vertical displacement.

If Ifl8 = 0, do not save vertical displacement.

If Ifl8 > 0, save vertical displacement.

Ifl9 is the output flag for critical head for no-delay interbeds printout for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl9 < 0, use default or previously defined settings of Ifl9 for printing critical head for no-delay interbeds.

If Ifl9 = 0, do not print critical head for no-delay interbeds.

If Ifl9 > 0, print critical head for no-delay interbeds.

Ifl10 is the output flag for saving critical head for no-delay interbeds to an unformatted disk file for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl10 < 0, use default or previously defined settings of Ifl10 for saving critical head for no-delay interbeds.

If Ifl10 = 0, do not save critical head for no-delay interbeds.

If Ifl10 > 0, save critical head for no-delay interbeds.

Ifl11 is the output flag for critical head for delay interbeds printout for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl11 < 0, use default or previously defined settings of Ifl11 for printing critical head for delay interbeds.

If Ifl11 = 0, do not print critical head for delay interbeds.

If Ifl11 > 0, print critical head for delay interbeds.

Ifl12 is the output flag for saving critical head for delay interbeds to an unformatted disk file for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl12 < 0, use default or previously defined settings of Ifl12 for saving critical head for delay interbeds.

If Ifl12 = 0, do not save critical head for delay interbeds.

If Ifl12 > 0, save critical head for delay interbeds.

Ifl13 is the output flag for volumetric budget for delay interbeds printout for the set of time steps specified by ISP1, ISP2, ITS1, and ITS2.

If Ifl13 < 0, use default or previously defined settings of Ifl13 for printing volumetric budget for delay interbeds.

If Ifl13 = 0, do not print volumetric budget for delay interbeds.

If Ifl13 > 0, print volumetric budget for delay interbeds.

IHM INTEGRATION WITH USG-T INPUT INSTRUCTIONS

IHM is the integrated Hydrologic Model (Ross and Geurink, 2018, Geurink et al., 2018) that dynamically combines HSPF (Bicknell et al., 2005) to simulate surface water hydrology (uplands with different land use / land cover features and soils and water bodies including lakes, reservoirs, wetlands, swamps, wet prairies, bogs, fens, etc.), with MODFLOW to simulate groundwater flow. USG-T includes this IHM integration capability and can therefore be used as the groundwater model for IHM. For an IHM simulation using USG-T, the USG-T executable must be included in the same directory as the IHM executable. Since the codes are independent of each other, any updates of USG-T will also contain the respective IHM integration modules and thus can be readily replaced as they become available. Note however, that all USG-T capabilities are not integrated into the IHM capabilities. The IHM details are provided by Geurink et al., (2018), while a brief summary of IHM capabilities and functionality is provided in the section on IHM Integration with USG-T in the GWT-v2 document.

Input/output formats and associated instructions for IHM integration are provided in this document. Input/output formats and details for the surface-water portions of IHM and for the integration of the groundwater and surface-water models can be found in Bicknell et al (2005) and Geurink et al. (2018), respectively. The IHM integration is not a separate package and therefore it is not accessed through the NAME file. Instead, input/output for the IHM integration is provided within the respective packages themselves, where the changes occur when information is passed between MODFLOW (USG-T) and the IHM.

Input of the keyword “IHM” (on the first line of data) in the BAS file indicates that the simulation is for an integrated hydrologic model and that the IHM interface routines will be invoked from within USG-T. The keyword is followed by a unit number for a file that writes USG-T debug information for an IHM simulation (in addition to similar information that is provided in the listing file).

IHM interacts with USG-T by using groundwater output information at each integration time-step for surface-water calculations, as well as by providing input to the groundwater model at each integration timestep. Therefore, at simulation startup and throughout the simulation, IHM writes many MODFLOW package files to update the groundwater input depending on surface-water model conditions. To avoid populating files that will be revised during startup of an IHM simulation, the modeler should use the guidelines found in the IHM User Guide (Geurink et al.,

2018) to determine general user input requirements for each package. The following subsection describes the procedure for running an IHM simulation with USG-T.

Running an IHM Simulation with USG-T

The following inputs are included in addition to the traditional USG-T inputs, for running an IHM simulation with USG-T as the groundwater model.

1. Model files for the groundwater portion of the IHM model are created in the standard manner as for any USG-T simulation. Generally, these files are ASCII text files and can be created using workflow approaches that put together elements of the model, or Graphical User Interfaces (GUIs) that accommodate MODFLOW-USG or USG-T groundwater models. To avoid preparing inputs that IHM will replace, refer to Section 6 of the IHM User Guide for details about minimum user-supplied inputs.
2. In addition to the regular USG-T input, for an IHM simulation, the BAS file includes a keyword “IHM” on the first line of data to indicate that the integration modules will be invoked. The keyword is followed by a number that identifies a Fortran Unit number (if greater than zero) on which IHM-specific debugging information for an IHM simulation is saved. If the Fortran Unit number is zero, then IHM-specific debugging information for the IHM run is not saved. NOTE: At simulation startup, IHM replaces user-supplied stress period count and rewrites the list of stress period records. Refer to Section 6 of the IHM User Guide for details about minimum user-supplied inputs.
3. If IHM debugging information is saved by having a positive Fortran Unit number after the “IHM” keyword in the BAS file, the NAME file should open the debugging output file under a DATA type using the same unit number as in the BAS file.
4. The NAME file of an IHM simulation can contain the optional keyword NO-ARCHIVE following the filename for any input or output file. In a MODFLOW simulation, information for all stress periods is required as input, and provided as output by default and all the data is considered as “Archived”. If the NO-ARCHIVE option is used to open a file, then information within that file will be “Replaced” at each stress period during the simulation and only the last stress period information will be retained. Thus, “Archived” input and output files will contain data for all stress periods of a simulation, while “Replaced” files will contain only data for the latest stress period. “Replaced” input data will only read the first stress period information since it is expected that the IHM portion of the code will update the information but not keep information from previous stress periods.
5. The NAME file should open a file “fname.SY” on a unique unit number under file type SYF (the file name and extension can be selected by the user). This file contains the specific yield (SY; secondary storage in MODFLOW terminology) for all cells in layer 1 of the model (or optionally, for all cells in convertible layers of the model, if the SY-ALL option is also invoked in the BAS file). During an IHM simulation at every integration time-step (i.e., MODFLOW stress period), the IHM updates SY values in the SYF file for layer 1 only (if SY-ALL option **not** used) or for all convertible layers (if SY-ALL option used). For layers not defined as convertible by LAYCON or LAYTYP, SY values do not exist in the SYF file. For a non-convertible layer that requires SY input, only the BCF or LPF file contains SY value(s). The magnitude of temporally-variable SY varies

with soil moisture and depth-to-water table. After IHM updates the SYF file with revised values for only convertible layers, USG-T reads the entire updated SYF file at every integration time-step (i.e., at the start of each MODFLOW stress period) to update SY for the upcoming stress period.

6. The RIV file can include the optional BINARY statement on the first line to indicate that river boundary data will be supplied from a separate file in binary formats. During an IHM simulation, the IHM portion of the code updates this RIV data at every integration time-step using river stages computed by IHM. Accounting for the file being either "Archived' or "Replaced", USG-T reads this updated data at every integration time-step. Since this information can be voluminous, use of a binary file by IHM quickens the data transfer. The "Archived" file structure is the default of IHM (and the way USG-T operates with reading and writing of all stress period information as requested). "Replaced" files are denoted by an optional keyword NO-ARCHIVE next to the filename in the model's NAME file. Refer to Section 6 of the IHM User Guide for details about minimum user-supplied inputs.
7. If binary RIV input is used, then a binary file with data for the RIV boundary should also be opened in the NAME file on the same Fortran Unit number as was supplied to the BINARY statement in the RIV input dataset.
8. IHM also writes new data to the RCH, EVT, and WEL files at every integration time-step. Refer to Section 6 of the IHM User Guide for details about minimum user-supplied inputs. Accounting for the file being either "Archived' or "Replaced", USG-T reads the new data for every integration time-step.
9. The IHM writes the entire GHB file at simulation startup. Refer to Section 6 of the IHM User Guide for details about minimum user-supplied inputs. USG-T reads data for one stress period for every integration time-step as is typical for a MODFLOW simulation.

An IHM run also requires that USG-T pause at the beginning of every integration time-step so that IHM can update data for the RCH, EVT, WEL, and RIV files and update data for the specific yield external file. Once IHM has done its computations and updates this data, it sends output to the screen, which is read by USG-T to continue the groundwater computation.

There are no known compatibility issues with running IHM using any of the USG-T capabilities and boundary conditions. For instance, the groundwater simulation of an integrated model may use the different formulations, boundary conditions, and other packages such as flow barriers (HFB Package) or conduit flow (CLN Package) seamlessly. This is because the implementation of IHM is modular with information being transferred between IHM and USG-T only at the start of each integration time-step in the main program. However, for an IHM run that uses USG-T packages which are not integrated into the IHM framework, mass balance closure cannot be evaluated and groundwater flows that should be integrated with surface-water flows could cause the results to be incomplete.

In the process of running an integrated hydrologic model, data in USG-T packages BAS, BCF, GHB, WEL, RCH, EVT, RIV, and OC are modified by IHM at simulation startup or at IHM integration time steps. Also, IHM uses information from the DIS (for a structured grid model), DISU (for an unstructured grid model), and CHD packages. Any MODFLOW package not specifically listed above within this paragraph that contains material properties could also be used instead of or in addition to BCF package. For instance, the material properties could be

augmented by using the Horizontal Flow Barrier (HFB) Package and/or provided by the Layer Property Flow (LPF) package instead of the BCF package. Also, any MODFLOW package not specifically listed above within this paragraph which produces a file representing mass (e.g., flow) to account for a portion of the simulated water balance could be included in an IHM simulation with the following caveats: (a) The IHM simulation and postprocessing codes require modification if the simulated mass should be integrated with uplands or water bodies via HSPF to account for the coupled influences of this water on the simulated system and to demonstrate water balance closure. (b) At a minimum to demonstrate water balance closure, the IHM water balance postprocessing code requires modification even when the simulated water does not require integration with uplands or water bodies via HSPF.

Specific-Yield (SYF) File

IHM updates SY values at every integration time-step (i.e., MODFLOW stress period), depending on soil moisture and depth to water table. The updated SY array is output to the SYF file which is then read by USGT prior to simulation for the next MODFLOW stress period. USGT expects an updated SYF array for layer 1 only, unless the SY-ALL option is selected in the BAS file in which case USGT expects an updated SYF array for all layers in the model which are convertible. Input for the SYF file is read from the file that has a filetype of "SYF" in the Name File.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

If *UNSTRUCTURED* option is used, then read item 1a.

1a. [SY(NDSLAY)] -- U1DREL

Otherwise, if *UNSTRUCTURED* option is not used then read item 1b for structured input

1b. [SY(NCOL,NROW)] -- U2DREL

Item 1 is the specific yield array for all cells in layer 1 by default. Item 1 is repeated for each convertible layer in the model grid if the SY-ALL option was selected in the BAS file.

Explanation of Variables Read by the SYF File:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The "#" character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

SY—is the specific yield array of layer 1 only by default. If the SY-ALL option is selected in the BAS file, then the SY array is read only for layers that are convertible (i.e., when LAYCON in the BCF file is 2, 3, or 4, or when LAYTYP in the LPF file is not zero).

Note that any of the MODFLOW options for reading arrays may be used by USGT to read array(s) within the SYF file (see section on input instructions for array reading utility subroutines). At a minimum, IHM will always change SY values for layer 1. When IHM does not change some SY values for a convertible layer (i.e., temporally-variable SY exception cases) it means the cell(s) are in a confined state or SY does not depend on soil moisture and

depth to water table (e.g., rock conditions). For temporally-variable SY exception cases, IHM uses the original values of SY as provided by the model developer in the BCF or LPF file and reproduces them in the SYF file with no change. See the IHM User Guide for instructions about preparation of the SYF file prior to an IHM simulation.

References

Bicknell, B.R., Imhoff, J.C., Kittle, Jr., J.L., Jobes, T.H., and Donigian, Jr., A.S. (2005). *Hydrological simulation program – FORTRAN: HSPF user's manual for Release 12.2*. U.S. Environmental Protection Agency, Athens, GA.

Geurink, J.S., Shelby, J.L., Murch, R., and Tara, P., 2018, Integrated Hydrologic Model Version 3 User Guide, Prepared for Tampa Bay Water and the Southwest Florida Water Management District, Brooksville, FL.

Ross, M.A. and Geurink J.S., 2018, Integrated Hydrologic Model Version 3 Theory and Implementation. Prepared for Tampa Bay Water, Clearwater, FL and the Southwest Florida Water Management District, Brooksville, FL.

GHOST NODE CORRECTION (GNC) PACKAGE INPUT INSTRUCTIONS

Input for the Ghost Node Correction (GNC) Package is read from the file that has file type "GNC" in the Name File. All variables are read in free format. The GNC package is not needed and is therefore inactivated, for a structured finite-difference grid. If the GNC contribution to sub-grid scale displacements for CLN nodes is required, the problem should be run as unstructured.

The GNC package allows for any user defined maximum number of adjacent contributing nodes and associated contributing fractions. If it is determined that unconfined simulations are more accurate with contributing factors that are function of the unconfined conductance, then the user can set the appropriate flag (IFLALPHAn = 1) and input effective saturated conductance instead of contributing factors for all the contributing nodes to the ghost node, and the code will internally compute the nonlinear contributing factors depending on the upstream water levels. This option may also be used for confined flow situations however, there is no benefit to doing so as the factors would be linear and constant.

FOR EACH SIMULATION

0. [#Text]

Item 0 is optional—"#" must be in column 1. Item 0 can be repeated multiple times.

1. NPGNCn MXGNn NGNCNPn MXADJn I2Kn ISYMGNCn IFLALPHAn ***[NOPRINT]***

The optional keyword “NOPRINT” specifies that lists of GNC cells will not be written to the Listing File.

2. [PARNAM PARTYP Parval NLST]

3. [NodeN NodeM (NodeJ, J=1,MXADJn) (FactorJ, J=1,MXADJn] FactorN

These variables are free format. Note that FactorN is not required and is ignored if IFLALPHAn = 0.

Repeat Items 2 and 3 NPGNCn times. Items 2 and 3 are not read if NPGNCn is negative or zero.

NLST repetitions of Item 3 are required; they are read by subroutine ULSTRD. (SFAC of the ULSTRD utility subroutine applies to FactorJ to each of the additional J contributing nodes).

4. NodeN NodeM (NodeJ, J=1,MXADJn) (AlphaJ, J=1,MXADJn) AlphaN

These variables are free format. Note that AlphaN is not required and is ignored if IFLALPHAn = 0.

5. NACTGNCn

6. Pname

NACTGNCn repetitions of Item 6 are read. Item 6 is not read if NACTGNCn is negative or zero.

Explanation of Variables Read by the GNC Package:

Text—is a character variable (199 characters) that starts in column 2. Any characters can be included in Text. The “#” character must be in column 1. Lines beginning with # are restricted to the first lines of the file. Text is written to the Listing File.

NPGNCn—is the number of ghost node parameters to be defined in Items 2 and 3. Note: A GNCn parameter must be defined in Items 2 and 3, and made active using Item 6, to have an effect in the simulation.

MXGNn—is the maximum number of GNC cells that will be defined using parameters.

NGNCNPn—is the number of GNC cells defined without using parameters.

MXADJn—is the maximum number of adjacent contributing nodes that will be present in the simulation. Every ghost node in the simulation will have entries for each of the adjacent contributing nodes. If a ghost node has less contributing nodes than this maximum, then additional dummy contributing nodes should be inserted with a contributing factor of zero. A

value of negative or zero cannot be used for the dummy node number. The dummy node number should be set as the node number of the cell on which the Ghost Node resides (*n*) or the node number of the cell to which flow occurs (*m*), so that the connectivity matrix is not expanded, the consequence of which would be a larger matrix requiring more storage.

I2Kn—is a flag indicating if second-order correction is also applied to the unconfined transmissivity term by using $\overline{h}$ to compute the transmissivity of node $\overline{n}$ instead of *h*.

If I2Kn = 0, second-order correction is not applied to the unconfined transmissivity term.

If I2Kn = 1, second-order correction is applied to the unconfined transmissivity term.

ISYMGNCn—is a flag indicating if the GNC formulation is applied in an implicit manner on the left-hand side matrix for an asymmetric system, or in an explicit manner on the right-hand side vector with iterative updates as is required for symmetric systems.

If ISYMGNCn = 0, use implicit update for asymmetric formulation.

If ISYMGNCn = 1, use explicit update for symmetric formulation.

IFLALPHAn—is a flag that indicates the meaning of input coefficients AlphaJ

If IFLALPHAn = 0, the coefficients AlphaJ represent the contributing factors α_j from all adjacent contributing nodes.

If IFLALPHAn = 1, the coefficients AlphaJ represent the saturated conductances between the ghost node location and node *j*, and the contributing factors are computed internally using the equations in the report for the unconfined conductances.

PARNAM—is the name of a parameter. This name can consist of 1 to 10 characters and is not case sensitive. That is, any combination of the same characters with different case will be equivalent.

PARTYP—is the type of parameter. For the GNC Package, the only allowed parameter type is GNC, which defines values of the ghost node coefficient of the cell.

Parval—is the parameter value. This parameter value may be overridden by a value in the Parameter Value File.

NLST—is the number of ghost node cells included in the parameter.

NodeN—is the node number of the cell in which the ghost node is located, $\overline{n}$.

NodeM—is the node number of the connecting cell, *m*, to which flow occurs from the ghost node $\overline{n}$.

NodeJ—is the node number of a contributing cell *j*, which contributes to the interpolated head value at the ghost node, $\overline{n}$. This Item is repeated for each of the MXADJn adjacent contributing cells of the ghost node. Note that if the number of adjacent contributing cells is less than MXADJn for any ghost node, then dummy node numbers should be inserted with an associated contributing factor of zero. As mentioned earlier, the dummy node number should be set as the node number of the cell on which the Ghost Node resides (*n*) or the node number of the cell to which flow occurs (*m*), so that the connectivity matrix is not expanded

FactorJ—is the factor used to calculate the contributing factor (α_j) from the parameter value. The term α_j is the product of FactorJ and the parameter value, for each of the J=1,MXADJn contributing nodes.

FactorN—is the factor used to calculate conductance between the ghost node and node n from the parameter value. The calculated conductance is the product of FactorN and the parameter value.

AlphaJ—is the contributing factor α_j of the ghost node. This Item is repeated for each of the **MXADJn—** adjacent contributing cells of the ghost node. Note that if the number of adjacent contributing cells is less than MXADJn for any ghost node, then dummy node numbers should be inserted with an associated contributing factor of zero. Also note that AlphaJ represents the conductance between cell *j* and the Ghost Node location when the flag IFLALPHAn=1.

AlphaN—is the conductance between the ghost node and node *n*. This value is used only if the flag IFLALPHAn=1.

NACTGNCn—is the number of active GNC parameters.

Pname—is the name of a parameter to be used in the simulation. NACTGNCn parameter names will be read.

SPARSE MATRIX SOLVER (SMS) PACKAGE INPUT INSTRUCTIONS

The SMS Package input instructions include flags, indices and tolerances for the nonlinear solution of the unconfined groundwater flow equation as well as for the matrix solution scheme selected for solution of the matrix equations. Guidance for selection of appropriate solution schemes is provided in the main document under the section “Guidance for Applying

MODFLOW-USG". Recommended values for of numerical parameters used by the SMS package are provided below. The input is read in as free format.

FOR EACH SIMULATION

1a. OPTIONS

1b. HCLOSE HICLOSE MXITER ITER1 IPRSMS NONLINMETH LINMETH [OPTIONS2]

If NONLINMETH ≠ 0 and OPTIONS is not specified then read item 2

2. THETA AKAPPA GAMMA AMOMENTUM NUMTRACK BTOL BREDUC RESLIM ITRUNCNEWTON

If LINMETH = 1 and OPTIONS is not specified then read item 3 for the χMD solver

3. IACL NORDER LEVEL NORTH IREDSYS RRCTOL IDROPTOL EPSRN

If LINMETH = 2 and options is not specified then read item 4 for the PCGU solver

4. [CLIN] IPC ISCL IORD RCLOSEPCGU

Explanation of Variables Read by the SMS Package:

OPTIONS— are keywords that activate default solver options:

SIMPLE indicates that default solver input values will be defined that work well for nearly linear models. This would be used for models that do not include nonlinear stress packages and models that are either confined or consist of a single unconfined layer that is thick enough to contain the water table within a single layer.

MODERATE indicates that default solver input values will be defined that work well for moderately nonlinear models. This would be used for models that include nonlinear stress packages and models that consist of one or more unconfined layers. The "MODERATE" option should be used when the "SIMPLE" option does not result in successful convergence.

COMPLEX indicates that default solver input values will be defined that work well for highly nonlinear models. This would be used for models that include nonlinear stress packages

and models that consist of one or more unconfined layers representing complex geology and sw/gw interaction. The “COMPLEX” option should be used when the “MODERATE” option does not result in successful convergence.

The values of solver parameters for the various options are shown below in Tables 1 and 2.

HCLOSE—is the head change criterion for convergence of the outer (nonlinear) iterations, in units of length. When the maximum absolute value of the head change at all nodes during an iteration is less than or equal to HCLOSE, iteration stops. Commonly, HCLOSE equals 0.01.

HICLOSE—is the head change criterion for convergence of the inner (linear) iterations, in units of length. When the maximum absolute value of the head change at all nodes during an iteration is less than or equal to HICLOSE, the matrix solver assumes convergence. Commonly, HICLOSE is set an order of magnitude less than HCLOSE.

MXITER—is the maximum number of outer (nonlinear) iterations -- that is, calls to the solution routine. For a linear problem MXITER should be 1.

ITER1—is the maximum number of inner (linear) iterations. The number typically depends on the characteristics of the matrix solution scheme being used. For nonlinear problems, ITER1 usually ranges from 60 to 600; a value of 100 will be sufficient for most linear problems.

IPRSMS—is a flag that controls printing of convergence information from the solver:

0 – print nothing

1 – print only the total number of iterations and nonlinear residual reduction summaries

2 – print matrix solver information in addition to above

NONLINMETH—is a flag that controls the nonlinear solution method and under-relaxation schemes

0 – Picard iteration scheme is used without any under-relaxation schemes involved

> 0 – Newton-Raphson iteration scheme is used with under-relaxation. Note that the Newton-Raphson linearization scheme is available only for the upstream weighted solution scheme of the BCF and LPF packages.

< 0 – Picard iteration scheme is used with under-relaxation.

The absolute value of NONLINMETH determines the underrelaxation scheme used.

1 or -1 – Delta-Bar-Delta under-relaxation is used.

2 or -2 – Cooley under-relaxation scheme is used.

Note that the under-relaxation schemes are used in conjunction with gradient based methods, however, experience has indicated that the Cooley under-relaxation and damping work well also for the Picard scheme with the wet/dry options of MODFLOW.

LINMETH—is a flag that controls the matrix solution method

1 – the χMD solver of Ibaraki (2005) is used.

2 – the unstructured pre-conditioned conjugate gradient solver of White and Hughes (2011) is used.

OPTIONS2— are keywords that activate solver specific options:

SOLVEACTIVE — indicates that the linear solvers will only solve for active model cells, i.e. model cells with IBOUND ≠ 0. With this option, matrices passed to the linear solver are compressed by ignoring all inactive (IBOUND=0) model cells. This option improves the simulation time in proportion to the number of inactive cells in the model. This option is recommended for models that have a large number of inactive model cells. This keyword, if invoked, should be added on the first line of this package before other optional keywords. This option is available with the χMD (LINMETH=1) and the PCGU (LINMETH=2) solvers.

DAMPBOT — indicates that the bottom damping procedure of MODFLOW-NWT will be applied to the solution. Note that the USGS release of MODFLOW-USG Version 1.4 includes this bottom averaging procedure as a default.

SHIFT — indicates that the right-hand vector will be translated before and after each linear solve. The shift amount is the old solution vector (HOLD for a flow solution or COLD for a transport solution). The solution vector is shifted back by that amount after calling the linear solver.

TRUNCATEDNEWTON — indicates that truncated Newton approach is to be used. The maximum cutoff fraction is set at a default of 0.9

TRUNCATEDNEWTONCUTOFF fraction — indicates that truncated Newton approach is to be used with the maximum cutoff fraction input as the "fraction" variable following the keyword. This is the upper limit residual fraction that is used for the residual cutoff (so the default of 0.9 means that the residual is limited to 90% of the previous residual). A smaller value (for instance 0.01) will incur more iterations of the linear solver to honor a smaller residual limit from the previous residual.

SOLVEROUTPUTFILE isolverfile — indicates that solver output will also be written to a separate file which is loaded on Fortran Unit "isolverfile" which is input following the "SOLVEROUTPUTFILE" keyword. Note that the NAMEFILE should also open the solver output file on the same unit number "isolverfile" used here.

THETA—is the reduction factor for the learning rate (under-relaxation term) of the delta-bar-delta algorithm. The value of THETA is between zero and one. If the change in the variable (head) is of opposite sign to that of the previous iteration, the under-relaxation term is reduced by a factor of THETA. The value usually ranges from 0.3 to 0.9; a value of 0.7 works well for most problems.

AKAPPA—is the increment for the learning rate (under-relaxation term) of the delta-bar-delta algorithm. The value of AKAPPA is between zero and one. If the change in the variable (head) is of the same sign to that of the previous iteration, the under-relaxation term is increased by an increment of AKAPPA. The value usually ranges from 0.03 to 0.3; a value of 0.1 works well for most problems.

GAMMA—is the history or memory term factor of the delta-bar-delta algorithm. Gamma is between zero and 1 but cannot be equal to one. When GAMMA is zero, only the most recent history (previous iteration value) is maintained. As GAMMA is increased, past history of iteration changes has greater influence on the memory term. The memory term is

maintained as an exponential average of past changes. Retaining some past history can overcome granular behavior in the calculated function surface and therefore helps to overcome cyclic patterns of non-convergence. The value usually ranges from 0.1 to 0.3; a value of 0.2 works well for most problems.

AMOMENTUM—is the fraction of past history changes that is added as a momentum term to the step change for a nonlinear iteration. The value of AMOMENTUM is between zero and one. A large momentum term should only be used when small learning rates are expected. Small amounts of the momentum term help convergence. The value usually ranges from 0.0001 to 0.1; a value of 0.001 works well for most problems.

NUMTRACK—is the maximum number of backtracking iterations allowed for residual reduction computations. If NUMTRACK = 0 then the backtracking iterations are omitted. The value usually ranges from 2 to 20; a value of 10 works well for most problems.

BTOL—is the tolerance for residual change that is allowed for residual reduction computations. BTOL should not be less than one to avoid getting stuck in local minima. A large value serves to check for extreme residual increases, while a low value serves to control step size more severely. The value usually ranges from 1.0 to 10^6; a value of 10^4 works well for most problems but lower values like 1.1 may be required for harder problems.

BREDUC—is the reduction in step size used for residual reduction computations. The value of BREDUC is between zero and one. The value usually ranges from 0.1 to 0.3; a value of 0.2 works well for most problems.

RESLIM—is the limit to which the residual is reduced with backtracking. If the residual is smaller than RESLIM, then further backtracking is not performed. A value of 100 is suitable for large problems and residual reduction to smaller values may only slow down computations.

For the χMD solver (Ibaraki, 2005)

IACL—is the flag for choosing the acceleration method.

0 – Conjugate Gradient – select this option if the matrix is symmetric.

1 – ORTHOMIN

2 - BiCGSTAB

NORDER—is the flag for choosing the ordering scheme.

0 – original ordering

1 – reverse Cuthill McKee ordering

2 – Minimum degree ordering

LEVEL—is the level of fill for ILU decomposition. Higher levels of fill provide more robustness but also require more memory. For optimal performance, it is suggested that a large level of fill be applied (7 or 8) with use of drop tolerance.

NORTH—is the number of orthogonalizations for the ORTHOMIN acceleration scheme. A number between 4 and 10 is appropriate. Small values require less storage but more iteration may be required. This number should equal 2 for the other acceleration methods.

IREDSYS—is the index for creating a reduced system of equations using the red-black ordering scheme.

0 – do not create reduced system

1 – create reduced system using red-black ordering

RRCTOL—is a residual tolerance criterion for convergence. The root mean squared residual of the matrix solution is evaluated against this number to determine convergence. The solver assumes convergence if either HICLOSE (the absolute head tolerance value for the solver) or RRCTOL is achieved. Note that a value of zero ignores residual tolerance in favor of the absolute tolerance (HICLOSE) for closure of the matrix solver.

IDROPTOL—is the flag to perform drop tolerance.

0 – do not perform drop tolerance

1 – perform drop tolerance

EPSRN—is the drop tolerance value. A value of 10^{-3} works well for most problems.

For PCGU Solver (White and Hughes, 2011)

CLIN— an option keyword that defines the linear acceleration method used by the PCGU solver.

CLIN = 'CG', preconditioned conjugate gradient method.

CLIN = 'BCGS', preconditioned bi-conjugate gradient stabilized method.

If CLIN is not specified the preconditioned conjugate gradient method is used. The preconditioned conjugate gradient method should be used for problems with a symmetric

coefficient matrix. The preconditioned biconjugate gradient stabilized method should be used for problems with a non-symmetric coefficient matrix (for example, with problems using the Newton-Raphson linearization scheme).

IPC— an integer value that defines the preconditioner.

IPC = 0, No preconditioning.

IPC = 1, Jacobi preconditioning.

IPC = 2, ILU(0) preconditioning.

IPC = 3, MILU(0) preconditioning.

IPC=3 works best for most problems.

ISCL is the flag for choosing the matrix scaling approach used.

0 –no matrix scaling applied

1 –symmetric matrix scaling using the scaling method by the POLCG preconditioner in Hill (1992).

2 –symmetric matrix scaling using the ℓ^2 norm of each row of **A** ($\mathbf{D}_R$) and the ℓ^2 norm of each row of $\mathbf{D}_R\mathbf{A}$.

ISCL must be 1 or 2 if the ILU(0) or MILU(0) preconditioners are used (IPC = 2 or 3) with matrix reordering (IORD > 0).

IORD is the flag for choosing the matrix reordering approach used.

0 – original ordering

1 – reverse Cuthill McKee ordering

2 – minimum degree ordering

If reordering is used, reverse Cuthill McKee ordering has been found to be a more effective reordering approach for the test problems evaluated.

RCLOSEPCGU—a real value that defines the flow residual tolerance for convergence of the PCGU linear solver. This value represents the maximum allowable residual at any single node. Value is in units of length cubed per time, and must be consistent with MODFLOW-USG length and time units. Usually a value of 1.0×10^{-1} is sufficient for the flow-residual criteria when meters and seconds are the defined MODFLOW-USG length and time.

SMS Output

Diagnostic output from the SMS package includes the solver iteration details (or summary), residual reduction information, and the nonlinear (outer) iteration summary. Residual reduction information includes the incoming and final accepted residuals, the backtracking count (IBCOUNT) and a flag (IBFLAG) indicating the backtracking status for each nonlinear iteration as indicated below.

IBFLAG

= 0 – backtracking was not performed

= 1 – backtracking was performed and the routine exited because the required residual reduction was achieved.

= 2 – backtracking was performed and the routine exited because the maximum number of backtracks, NUMTRACK was exceeded.

=3 – backtracking was performed and the routine exited because the new residual was less than the residual reduction limit, RES_LIM.

=4 – backtracking was performed and the routine exited because the largest step-size was less than the convergence limit of HCLOSE.

The residual reduction information is provided if the solver print-flag IPRSMS is greater than or equal to one.

The nonlinear iteration summary includes the total number of nonlinear iterations required for convergence and the maximum head change at each nonlinear iteration (immediately after a matrix solve), along with the node number where the maximum head change occurs. This information, along with the backtracking information may be used to tune the parameters for the delta-bar-delta algorithm and the residual reduction scheme to obtain convergence or improve robustness of the simulations. The summary at each iteration of the matrix solver is also provided in the output, if the value of IPRSMS is equal to two. This information is useful in tuning solver behavior if the matrix solver is stalling or failing.

Table 1. *Parameter Values for the Various Default XMD Solver Options*

Parameter	Option		
	Simple	Moderate	Complex
IACL	1	2	2
NORDER	0	0	1
LEVEL	3	3	5
NORTH	5	5	7
IREDSYS	1	1	1
IDROPTOL	0	1	1
RRCTOL	0.00E+00	0.00E+00	0.00E+00
EPSRN	1.00E-03	1.00E-03	1.00E-05
THETA	1.00E+00	9.00E-01	8.00E-01
AKAPPA	0.00E+00	1.00E-04	1.00E-04
GAMMA	0.00E+00	0.00E+00	0.00E+00
AMOMENTUM	0.00E+00	0.00E+00	0.00E+00
NUMTRACK	0	0.00E+00	2.00E+01
BTOL	0.00E+00	0.00E+00	1.05E+00
BREDUC	0.00E+00	0.00E+00	1.00E-01
RES_LIM	0.00E+00	0.00E+00	2.00E-03

Table 2. *Parameter Values for the Various Default PCGU Solver Options*

Parameter	Option		
	Simple	Moderate	Complex
IPC	2	2	2
ISCL	2	2	2
IORD	2	2	2
RCLOSEPCGU	1.00E-04	1.00E-04	1.00E-04
THETA	1.00E+00	9.00E-01	8.00E-01
AKAPPA	0.00E+00	1.00E-04	1.00E-04
GAMMA	0.00E+00	0.00E+00	0.00E+00

AMOMENTUM	0.00E+00	0.00E+00	0.00E+00
NUMTRACK	0	0.00E+00	2.00E+01
BTOL	0.00E+00	0.00E+00	1.05E+00
BREDUC	0.00E+00	0.00E+00	1.00E-01
RES_LIM	0.00E+00	0.00E+00	2.00E-03

GRID SPECIFICATION FILE (GSF) INPUT INSTRUCTIONS

The GSF file formats below have been developed by John Doherty and are also used by PEST.

The control volume finite difference approach used in MODFLOW-USG does not require grid coordinate locations for its computations. However, grid coordinate locations are required for determining positions in space for combining geostatistical approaches with modeling. The grid specification file (GSF) provides details on the coordinates of a MODFLOW-USG grid and the vertices of each cell to assist with providing spatial locations to the grid blocks and with visualization of a grid. The following format for a GSF file is suggested for use with USG-Transport simulations, which is compatible with geostatistical approaches developed in the parameter estimation software PEST and with several of the Graphical User Interfaces used by USG-Transport.

Line 1:

"STRUCTURED" or "UNSTRUCTURED"

If UNSTRUCTURED then

Line 2:

nnode nlay iz ic

where:

nnode is the number of nodes in the grid

nlay is the number of layers in the model.

iz is 1 if elevations of node and mesh element vertices are supplied; 0 otherwise

ic is 1 if the cell specifications associated with each node are supplied; 0 otherwise

If IC is supplied as 1

A list of cell vertex coordinates is now provided. These vertices can be cited by index later in this file.

where mesh geometric details are provided. The indices of vertices are defined implicitly by their positions in the following list.

Line 3:

nvertex is the number of element vertex definitions to follow

NVERTEX next lines:

x, y, z

where:

x, y and z are the coordinates of each element vertex

If IZ is 1 and IC is 1 then:

NNODE next lines:

inode x y z lay m (ivertex(i),i=1,m)

where:

inode is a node number

x, y and z are node coordinates

lay is the layer number of the node

m is the number of vertices defining the three-dimensional element associated with the node

ivertex are node indices defined with reference to the node list provided above

Or if IZ is 0 and IC is 0 then:

NNODE next lines:

inode x y lay

Or if IZ is 1 and IC is 0 then:

NNODE next lines:

inode x y z lay

Or if IZ is 0 and IC is 1 then:

NNODE next lines:

inode x y lay m (x(i), y(i), i=1,m)

Or if STRUCTURED then

Line 2:

nrow ncol nlay

where:

nrow, ncol and nlay are the number of rows, columns and layers in the structured grid

Line 3:

CORNERCODE e0 n0 rotation

where:

CORNERCODE is1 for top left of grid; 2 for bottom left of grid

e0 and n0 are east and north coordinates for the identified corner

rotation is the angle between east and the grid row direction (positive for anticlockwise)

Line 4 (and then wrapped):

(delr(icol), icol=1,ncol)

where:

delr is an array of cell widths in the row direction

Next line (and then wrapped):

(delc(irow),irow=1,nrow)

where

delc is an array of cell widths in the column direction

Next line:

<EOF> or ELEVCODE

where:

ELEVCODE is an integer which is 0 (equivalent to <EOF>) or 1 or 2

If ELEVCODE is 1 then

Next lines:

top_of_layer_1_array

bottom_of_layer_1_array

bottom_or_layer_2 array

etc

If ELEVCODE is 2 then

Next lines:

top_of_layer_1_array

bottom_of_layer_1_array

top_of_layer_2_array

bottom_of_layer_2_array

etc