

DATA INPUT INSTRUCTIONS FOR GROUND-WATER TRANSPORT PROCESS (GWT) Version (GWF1.16/GWT1.9)

The solute-transport simulation package that is integrated with MODFLOW-2000 is called the Ground-Water Transport Process (GWT). It is derived directly from the *MOC3D* model (Konikow and others, 1996), which had been integrated with MODFLOW-96 (Harbaugh and McDonald, 1996). Following is a set of instructions for preparing an input data set for the **GWT** process. For more comprehensive descriptions of input parameters, options, and underlying assumptions, the user should also refer to Konikow and others (1996), Kipp and others (1998), Goode (1999), and Heberton and others (2000).

One major change that has been implemented since the release of MOC3D Version 3.5 is the elimination of former item 18a, which was used to define the thickness of layers. This is no longer used because vertical discretization (and hence thickness) is now defined in the input data for MODFLOW-2000 (see Harbaugh and others, 2000). Another change is in the file type used in the MODFLOW name file. This version of the code is also compatible with the Lake and Gage Packages, the Constant-Head Boundary Package, the Streamflow-Routing Package, the Multi-Node Well Package, and the Drain-Return Package. [New information is shown in blue.](#)

***MODFLOW* Name File**

Transport simulation is activated by including a record in the *MODFLOW* name file using the file type (Ftype) “GWT” to link to the transport name file. The transport name file specifies the files to be used when simulating solute transport in conjunction with a simulation of ground-water flow using *MODFLOW*. The transport name file works in the same way as the *MODFLOW* name file. (The Ftype “CONC” is not valid with MODFLOW-2000.)

***MODFLOW* Source and Sink Packages**

Except for recharge and lakes, concentrations associated with fluid sources (C') are read as auxiliary parameters in the *MODFLOW* source package. The source concentration is read from a new column appended to the end of each line of the data file describing a fluid sink/source (see documentation for revised *MODFLOW* model; Harbaugh and McDonald, 1996a and 1996b). For example, concentrations associated with well nodes should be appended to the line in the WEL Package where the well's location and pumping rate are defined. These concentrations will be read if the auxiliary parameter “CONCENTRATION” (or “CONC”) appears on the first line of the well input data file. The concentration in recharge is defined separately, as described in a following section, “Source Concentration in Recharge File.” The preparation of input data files for using the Lake Package when solute-transport is also simulated is described in detail in the Lake Package documentation (Merritt and Konikow, 2000). [The preparation of input data files for using the Streamflow-Routing Package \(SFR2\) when solute-transport is also simulated is described in detail in the SFR2 documentation \(Niswonger and Prudic, 2005\).](#) [The preparation of input data files for using the Multi-Node Well Package](#)

(MNW) when solute transport is also simulated is described in detail by Konikow and Hornberger (2006).

In *MODFLOW*, fluid sources and sinks are treated numerically as being effectively distributed throughout the volume of the cell. Some fluxes, however, actually represent flow across the aquifer boundary (for example, recharge typically represents flux into the aquifer across the top boundary of the aquifer—usually the top face of a cell in the uppermost active layer in the model). Representing such a recharge flux as a distributed source term would be consistent with having a vertical velocity of zero on the top face. In the presence of recharge, however, the vertical velocity at the water table boundary is actually nonzero. *MODPATH* recognizes this inconsistency and allows the user to specify that certain fluxes represent boundary fluxes, and it then assigns that flux to the appropriate or assigned face. For example, recharge would be assigned to the top face of a cell, and the velocity on that face would be computed as the recharge flux divided by the effective porosity of the cell. The difference between these two conceptualizations would affect interpolation results for estimating the velocity and pathline of a particle in a boundary cell. Thus, it would also affect concentrations calculated using GWT. Therefore, the GWT model has implemented an option to assign fluxes on boundaries in the same manner as in *MODPATH*. This is implemented by using the new boundary flux input file (Ftype “bflx”) and (or) using the auxiliary parameter IFACE in list directed sink/source packages for *MODFLOW*.

To simulate solute transport the *MODFLOW* option enabling storage of cell-by-cell flow rates for each fluid source or sink is required in all fluid packages except recharge. The key word “CBCALLOCATE” (or “CBC”) must appear on the first line of each input data file for a fluid package (see Harbaugh and McDonald, 1996a and 1996b).

GWT Input Data Files

All input variables are read using free formats, except as specifically indicated. In free format, variables are separated by one or more spaces or by a comma and optionally one or more spaces. Blank spaces are not read as zeros. Variables that are optional are enclosed in brackets, as in {option}.

Ground-Water Transport Name File (GWT)

FOR EACH SIMULATION:

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1. Data:   FTYPE   NUNIT   FNAME
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The name file consists of records defining the names and unit numbers of the files. Each “record” consists of a separate line of data. There must be a record for the listing file and for the main *GWT* input file.

The listing (or output) file (“CLST”) must be the first record. The other files may be in any order. Each record can be no more than 79 characters.

FTYPE The file type, which may be one of the following character strings:

CLST GWT listing file (separate from the *MODFLOW* listing file) *[required]*.

MOC, MOCIMP, ELLAM Main GWT input data file *[required]*. Specifying **MOC** indicates dispersion calculations will be explicit (as described by Konikow and others, 1996); specifying **MOCIMP** indicates dispersion calculations will be implicit (as described by Kipp and others, 1998); and specifying **ELLAM** indicates that the solute-transport equation will be solved using the *ELLAM* method (as described by Heberton and others, 2000).

CRCH Concentrations in recharge *[optional]*.

CNCA Separate output file containing concentration data in ASCII (text-only) format *[optional]*. Frequency and format of printing controlled by NPNTCL and ICONFM. If concentrations are written to a separate output file, they will not be written to the main output file.

CNCB Separate output file containing concentration data in binary format *[optional]*.

VELA Separate output file with velocity data in ASCII format *[optional]*. Frequency and format of printing controlled by NPNTVL and IVELFM.

VELB Separate output file with velocity data in binary format *[optional]*.

PRTA Separate output file with particle locations printed in ASCII format *[optional]*. Frequency and format of printing controlled by NPNTPL.

PRTB Separate output file with particle locations printed in binary format *[optional]*.

P RTP Presence of this file type is a flag to indicate that the *z*-location of printed particle locations for PRTA and (or) PRTB options will be adjusted for changes in water-table elevation (and saturated thickness) relative to cell dimensions. This will allow plotting packages, such as Model Viewer (Hsieh and Winston, 2002), to accurately plot relative position of particles within cells in which the saturated thickness has changed. Only specify if PRTA or PRTB is active. A data file, filename, and unit number needs to be associated with this file type; however the file does not need to include any data. *[optional]*.

OBS Observation wells input file *[optional]*.

DATA For formatted files such as those required by the OBS package and for array data separate from the main GWT input data file *[optional]*.

DATA (BINARY) For formatted input/output files *[optional]*.

AGE Ground-water age simulation input file *[optional]*. (Compatibility with the *ELLAM* option has been incorporated in this new release.)

DP Double porosity input file *[optional]*. (Not compatible with *ELLAM* option.)

DK Simple reactions (decay, zero-order growth, retardation) input file *[optional]*. (Not compatible with *ELLAM* option.)

CHFB Transport properties for Horizontal Flow Barriers and alternate calculation of dispersive flux near HFB cells *[optional]*. This option only should be used if the HFB Package is active.

BFLX	Input file to convert certain distributed source/sink fluxes (recharge, evapotranspiration, and constant-head cells) to boundary fluxes <i>[optional]</i> .
CBDY	Input file to specify spatially varying source concentrations in horizontal or vertical flow across boundaries of a transport subgrid <i>[optional]</i> .
SSTR	Input file to specify that transient transport calculations will begin after the first stress period of the flow simulation <i>[optional]</i> .
MNWO	Input file to designate a multi-node well for observation of changes in concentration and other related data, as described by Konikow and Hornberger (2006) <i>[optional]</i> . This option only should be used if the MNW Package is active.
NUNIT	The FORTRAN unit number used to read from and write to files. Any legal unit number other than 97, 98, and 99 (which are reserved by <i>MODFLOW</i>) can be used provided that it is not previously specified in the <i>MODFLOW</i> name file.
FNAME	The name of the file.

Note: AGE, DP, and DK file types are described by Goode (1999). The CHFB file type is described by Hornberger and others (2002).

Files of type DATA and DATA(BINARY) can be designated as either input or output files. One of the options (either “OLD” for an input file or “REPLACE” for an output file) may be placed after the file name on the line listing the file type, unit number, and file name. If “OLD” is specified, the file must exist when the program is started. If “REPLACE” is specified and the file exists when the program is started, the existing file is deleted, then opened. The status of each file (“OLD”, “REPLACE”, or “UNKNOWN”) is now shown in the output file. Note that the “OLD” or “REPLACE” option is not required. If neither is listed, the file status is shown as “UNKNOWN” and program execution continues normally. When output to a BINARY file from an earlier model run exceeds the amount of output generated by the current model run, specifying “REPLACE” may be required to ensure the file does not include output from the previous run after the output generated by the current run. The options may be entered in any combination of uppercase and lowercase letters.

Main GWT Package Input (*MOC*, *MOCIMP*, or *ELLAM*)

Input for the solute-transport package is read from the unit specified in the transport name file. The input consists of up to 19 separate items, as described in detail below (note that item numbers do not necessarily correspond with line numbers in the file). These data are used to specify information about the transport subgrid, physical and chemical transport parameters, numerical solution variables, and output formats. Output file controls for the *GWT* package are specified in the transport name file, described previously.

FOR EACH SIMULATION:

1. Data: HEDMOC A two-line character-string title describing the simulation (80 text characters per line).
2. Data: HEDMOC (continued)
3. Data: ISLAY1 ISLAY2 ISROW1 ISROW2 ISCOL1 ISCOL2

ISLAY1 Number of first (uppermost) layer for transport.
 ISLAY2 Last layer for transport.
 ISROW1 First row for transport.
 ISROW2 Last row for transport.
 ISCOL1 First column for transport.
 ISCOL2 Last column for transport.

Notes:

Transport may be simulated within a subgrid, which is a “window” within the primary *MODFLOW* grid used to simulate flow. Row and column numbers specified here are those in the *MODFLOW* grid. Within the subgrid, the row and column spacing must be uniform if *FTYPE MOC* or *MOCIMP* are specified in the transport name file, but subgrid spacing can vary as in *MODFLOW* if *ELLAM* is specified. The thickness can vary from cell to cell and layer to layer. However, the range in thickness values (or product of thickness and porosity) should be as small as possible.

4. Data: NODISP DECAFY DIFFUS

NODISP Flag for no dispersion (set NODISP = 1 if no dispersion in problem; this will reduce storage allocation; in most cases, NODISP = 0).
 DECAFY First-order decay rate [1/T] (DECAFY = 0.0 indicates no decay occurs).
 DIFFUS Effective molecular diffusion coefficient [L^2/T].

Notes:

The decay rate (λ) is related to the half life ($t_{1/2}$) of a constituent by $\lambda = (\ln 2)/t_{1/2}$.

The effective molecular diffusion coefficient (D_m) includes the effect of tortuosity.

IF Ftype *MOC* OR *MOCIMP* IS ACTIVE:

- 5a. Data: NPMAX NPTPND

NPMAX Maximum number of particles available for particle tracking of advective transport in *GWT*. If set to zero, the model will calculate NPMAX according to the following equation:

$$NPMAX = 2 \times NPTPND \times NSROW \times NSCOL \times NSLAY.$$

NPTPND Initial number of particles per cell in transport simulation (that is, at $t = 0.0$). Valid options for default geometry of particle placement include 1, 2, 3, or 4 for one-dimensional transport simulation; 1, 4, 9, or 16 for two-dimensional transport simulation; and 1, 8, or 27 for three-dimensional transport simulation. The user can also customize initial placement of particles by specifying **NPTPND** as a negative number, in which case the minus sign is recognized as a flag to indicate custom placement is desired. In this case, the user must input local particle coordinates as described below.

IF Ftype *ELLAM* IS ACTIVE:

5b. Data: NSCEXP NSREXP NSLEXP NTEXP

NSCEXP Exponent used to calculate the number of subcells in the column direction (NSC, where $NSC = 2^{*}NSCEXP$).

NSREXP Exponent used to calculate the number of subcells in the row direction (NSR).

NSLEXP Exponent used to calculate the number of subcells in the layer direction (NSL).

NTEXP Exponent used to calculate the number of sub-time steps per transport time increment (NT).

Notes:

In general, numerical accuracy will be increased by increasing the value of these parameters. This will also, however, increase computational costs. For each of the four parameters above, the value represents the exponent y in the expression 2^y .

Entering a zero or negative value for any of the above variables will cause the code to use default values. Default values for **NSCEXP**, **NSREXP**, and **NSLEXP** are 2 in active dimensions and 1 in inactive dimensions (for example, if a simulation represented a two-dimensional areal problem in which the number of rows and columns were greater than one and the number of layers equals one, then default settings would be **NSCEXP** = 2, **NSREXP** = 2, and **NSLEXP** = 1, and the number of subcells in each direction would be 4, 4, and 2, respectively). The default value of **NTEXP** is 2.

IF **5a** IS READ AND *NPTPND* IS NEGATIVE IN SIGN:

6. Data: PNEWL PNEWR PNEWC

PNEWL Relative position in the layer (z) direction for initial placement of particle within any finite-difference cell.

PNEWR Relative position in the row (y) direction for initial placement of particle.

PNEWC Relative position in the column (x) direction for initial placement of particle.

Notes:

The three new (or initial) particle coordinates are entered sequentially for each of the **NPTPND** particles. Each line contains the three relative local coordinates for the new particles, in order of layer, row, and column. There must be **NPTPND** lines of data, one for each particle. The local coordinate

system range is from -0.5 to 0.5, and represents the relative distance within the cell about the node location at the center of the cell, so that the node is located at 0.0 in each direction.

FOR EACH SIMULATION:

7. Data: CELDIS {FZERO} {INTRPL}

- CELDIS Maximum fraction of cell dimension that particle may move in one step (typically, $0.5 \leq \text{CELDIS} \leq 1.0$). For *ELLAM*, CELDIS can be greater than 1.0, and specifying CELDIS = 0.0 will result in one transport time step being used (which is not generally recommended).
- FZERO If the fraction of active cells having no particles exceeds FZERO, the program will automatically regenerate an initial particle distribution before continuing the simulation (typically, $0.01 \leq \text{FZERO} \leq 0.05$). Do not specify if *ELLAM* is active.
- INTRPL Flag for interpolation scheme used to estimate velocity of particles. The default (INTRPL = 1) will use a linear interpolation routine; if INTRPL = 2, a scheme will be implemented that uses bilinear interpolation in the row and column (*j* and *i*) directions only (linear interpolation will still be applied in the *k*, or layer, direction). Do not specify if *ELLAM* is active, in which case the code will automatically set INTRPL = 1.

IF *MOCIMP* IS ACTIVE:

7.1 Data: FDTMTH NCXIT IDIREC EPSSLV MAXIT

- FDTMTH Weighting factor for temporal differencing of dispersion equation ($0.0 \leq \text{FDTMTH} \leq 1.0$). We suggest using either a value of FDTMTH = 0.5, a centered-in-time (or Crank-Nicolson) approximation, or FDTMTH = 1.0, a backward-in-time (or fully implicit) approximation. [Default value = 1]
- NCXIT Number of iterations for the explicitly-lagged cross-dispersive flux terms ($\text{NCXIT} \geq 1$). We suggest that the user initially specify a value of 2, but if the solution exhibits significant areas of negative concentrations, then the value of NCXIT should be increased to require more iterations, which typically will reduce the extent and magnitude of negative concentrations (at the cost of increased computational time). [Default value = 2]
- IDIREC Direction index for permutation of the red-black node renumbering scheme. The order is as follows: 1: x,y,z; 2: x,z,y; 3: y,x,z; 4: y,z,x; 5: z,x,y; and 6: z,y,x. The first direction index is advanced most rapidly and the last direction index is advanced least rapidly. In some cases, there can be a significant variation in the number of iterations needed to achieve convergence, depending on the order of the directions for the red-black renumbering. We suggest that the user initially specify IDIREC = 1. If this leads to a relatively large number of iterations (more than 10), then the user should experiment with alternate choices to determine the one

requiring the fewest number of iterations for their particular problem. [Default value = 1]

- EPSSLV Tolerance on the relative residual for the conjugate-gradient solution of the matrix of the difference equations. We suggest that the user initially specify $EPSSLV \leq 10^{-5}$. An adequately small value of EPSSLV has the property that a smaller value does not change the numerical solution within the number of significant digits desired by the user. In the single-precision code implemented here, EPSSLV should not be less than 10^{-7} . [Default value = 10^{-5}]
- MAXIT Maximum number of iterations allowed for the iterative solution to the difference equations for dispersive transport. In most cases, MAXIT = 100 is satisfactory. [Default value = 100]

Notes:

Entering a zero or out-of-range value for any of these five variables will cause the code to use the indicated default value.

FOR EACH SIMULATION:

8. Data: NPNTCL ICONFM NPNTVL IVELFM NPNTDL IDSPFM {NPNTPL}

- NPNTCL Flag for frequency of printing concentration data. If NPNTCL = -2, concentration data will be printed at the end of every stress period; if NPNTCL = -1, data will be printed at the end of every flow time step; if NPNTCL = 0, data will be printed at the end of the simulation; if NPNTCL = N > 0, data will be printed every Nth particle moves, and at the end of the simulation. Initial concentrations are always printed. Solute budget and mass balance information are only printed every time concentration data are saved.
- ICONFM Flag for output format control for printing concentration data. If concentration data are written to main output file (file type CNCA is not used), ICONFM represents a code indicating the format style (table 1, also see Harbaugh and McDonald, 1996a, p. 19). If concentration data are written to a separate output file (file type CNCA exists), specifying $ICONFM \geq 0$ will indicate that concentration data are to be written as a matrix of values for each layer of the subgrid, whereas specifying $ICONFM < 0$ will indicate that concentration data are to be written as a table of values having one row for each node in the subgrid and four columns (x , y , z , and concentration), where x , y , and z are the actual nodal coordinates in the length units of the model simulation. In both cases for an external file, values are written using a format of (1P10E12 . 4). Note that we follow the *MODFLOW* convention in that y increases from top to bottom row, and z increases from top layer to bottom layer. Also note that the x and y values are given with respect to the entire *MODFLOW* grid, but the z location is calculated only for vertical distances within the layers of the transport subgrid. If data are written in matrix style, one header line precedes and identifies the data for each layer. If data are written as a table of values, one header line is written each time that concentration data are saved.

- NPNTVL Flag for printing velocity data. If NPNTVL = -1, velocity data will be printed at the end of every stress period; if NPNTVL = 0, data will be printed at the end of the simulation; if NPNTVL > 0, data will be printed every Nth flow time steps, and at the end of the simulation.
- IVELFM Specification for format of velocity data, if being printed in main output file (see table 1).
- NPNTDL Flag for printing dispersion equation coefficients that include cell dimension factors (see section “Program Segments”). If NPNTDL = -2, coefficients will be printed at the end of every stress period; if NPNTDL = -1, coefficients will be printed at the end of the simulation; if NPNTDL = 0, coefficients will not be printed; if NPNTDL > 0, coefficients will be printed every Nth flow time step.
- IDSPFM Specification for format of dispersion equation coefficients (see table 1).
- NPNTPL Flag for printing particle locations in a separate output file (**only read** if file types “PRTA” or “PRTB” appear in the *GWT* name file). If either “PRTA” or “PRTB” is entered in the name file, initial particle locations will be printed to the separate file first, followed by particle data at intervals determined by the value of NPNTPL. If NPNTPL = -2, particle data will be printed at the end of every stress period; if NPNTPL = -1, data will be printed at the end of every flow time step; if NPNTPL = 0, data will be printed at the end of the simulation; if NPNTPL > 0, data will be printed every Nth particle moves, and at the end of the simulation. Only specify if *MOC* or *MOCIMP* is active.

Table 1. Formats associated with print flags. (Positive values for wrap format; negative values for strip format. Also see Harbaugh and McDonald, 1996, p. 19.)

Print flag	Format	Print flag	Format	Print flag	Format
0	10G11.4	7	20F5.0	14	10F6.1
1	11G10.3	8	20F5.1	15	10F6.2
2	9G13.6	9	20F5.2	16	10F6.3
3	15F7.1	10	20F5.3	17	10F6.4
4	15F7.2	11	20F5.4	18	10F6.5
5	15F7.3	12	10G11.4		
6	15F7.4	13	10F6.0		

FOR EACH SIMULATION:

- 9. Data: CNOFLO Concentration associated with inactive cells of subgrid (used for output purposes only).

FOR EACH LAYER OF THE TRANSPORT SUBGRID:

- 10. Data: CINT (NSCOL, NSROW) Initial concentration.
Module: U2DREL*

* Module is a standard *MODFLOW* input/output module.

FOR EACH SIMULATION, ONLY IF TRANSPORT SUBGRID DIMENSIONS ARE SMALLER THAN FLOW GRID DIMENSIONS, **AND ONLY IF *CBDY* PACKAGE IS INACTIVE:**

11. Data: CINFL (ICINFL) C' to be associated with fluid inflow across the boundary of the subgrid.
Module: UIDREL*

Notes:

The model assumes that the concentration outside of the subgrid is the same within each layer, so only one value of CINFL is specified for each layer within and adjacent to the subgrid. That is, the size of the array (ICINFL) is determined by the position of the subgrid with respect to the entire (primary) *MODFLOW* grid. If the transport subgrid has the same dimensions as the flow grid, this parameter should not be included in the input data set. If the subgrid and flow grid have the same number of layers, but the subgrid has fewer rows or fewer columns, ICINFL = NSLAY. Values are also required if there is a flow layer above the subgrid and/or below the subgrid. The order of input is: C' for first (uppermost) transport layer (if required); C' for each successive (deeper) transport layer (if required); C' for layer above subgrid (if required); and C' for layer below subgrid (if required). **The *CBDY* Package provides the flexibility to specify spatially varying values of CINFL.**

FOR EACH SIMULATION:

12. Data: NZONES Number of zone codes among fixed-head nodes in transport subgrid.
IF NZONES > 0:

Data: IZONE ZONCON
IZONE Value identifying a particular zone.
ZONCON Source concentration associated with nodes in the zone defined by IZONE above.

Notes:

Zones are defined within the IBOUND array in the BAS Package of *MODFLOW* by specifying unique negative values for fixed-head nodes to be associated with separate fluid source concentrations. Each zone is defined by a unique value of IZONE and a concentration associated with it (ZONCON). There must be NZONES lines of data, one for each zone. Note that values of IZONE in this list must be negative for consistency with the definitions of fixed-head nodes in the IBOUND array in the BAS Package. If a negative value of IBOUND is defined in the BAS package but is not assigned a concentration value here, *GWT* will assume that the source concentrations associated with those nodes equal 0.0.

If heads or source concentrations associated with fixed-head cells vary with time, the CHD or FHB packages should be used to simulate those cells and to specify the associated source concentrations using auxiliary variables. If the source concentration value for a given fixed-head cell is specified both here (in data set 12) and in CHD or FHB, the latter values will override the former values.

* Module is a standard *MODFLOW* input/output module.

FOR EACH LAYER OF THE TRANSPORT SUBGRID IF *MOC* OR *MOCIMP* IS ACTIVE:

13. Data: IGENPT (NSCOL, NSROW) Flag to treat fluid sources and sinks as either “strong” or “weak.”
Module: U2DINT*

Notes:

Where fluid source is “strong,” new particles are added to replace old particles as they are advected out of that cell. Where a fluid sink is “strong,” particles are removed after they enter that cell and their effect accounted for. Where sources or sinks are weak, particles are neither added nor removed, and the source/sink effects are incorporated directly into appropriate changes in particle positions and concentrations. If IGENPT = 0, the node will be considered a weak source or sink; if IGENPT = 1, it will be a strong source or sink. See section on “Special Problems” and discussion by Konikow and Bredehoeft (1978). This data set is skipped if *ELLAM* is active.

IF *NODISP* ≠ 1 (If dispersion is included in simulation):

14. Data: ALONG (NSLAY) Longitudinal dispersivity.
Module: U1DREL*
15. Data: ATRANH (NSLAY) Horizontal transverse dispersivity.
Module: U1DREL*
16. Data: ATRANV (NSLAY) Vertical transverse dispersivity.
Module: U1DREL*

Notes:

Items 14-16 should include one value for each layer in subgrid.

FOR EACH SIMULATION:

17. Data: RF (NSLAY) Retardation factor (RF = 1 indicates no retardation).
Module: U1DREL*

Notes:

If RF = 0.0 in input, the code automatically resets it as RF = 1.0 to indicate no retardation.

FOR EACH LAYER OF TRANSPORT SUBGRID:

18. Data: POR (NSCOL, NSROW) Cell porosity.
Module: U2DREL*

Notes:

The porosity is input as a separate array for each layer of the transport subgrid. The product of thickness and porosity should not be allowed to vary greatly among cells in the transport subgrid.

* Module is a standard *MODFLOW* input/output module.

Source Concentration in Recharge File (CRCH)

Concentrations in recharge, if the recharge package is used, are read from a separate unit specified in the *GWT* name file. This is defined using the file type (Ftype) “CRCH.”

FOR EACH STRESS PERIOD, IF RECHARGE PACKAGE USED:

1. Data: INCRCH Flag to reuse or read new recharge concentrations.

Notes:

Read new recharge concentrations if $INCRCH \geq 0$. Reuse recharge concentrations from the last stress period if $INCRCH < 0$.

2. Data: CRECH (NSCOL, NSROW) Source concentration associated with fluid entering the aquifer in recharge.
Module: U2DREL*

Transport Boundary Flux File (BFLX)

Options to specify recharge, evapotranspiration, and specific constant-head fluxes as representing a boundary flux rather than a distributed flux are read from a separate unit specified in the *GWT* name file for ftype “BFLX.”

In the same manner as in *MODPATH*, the user can choose to have all recharge applied (1) as a distributed source/sink term (which yields a zero flux and zero velocity condition on the top face of recharge cells), or (2) as a boundary flux (which, as in *MODPATH*, assigns the recharge flux as inflow across the top face of recharge cells). Similarly, the user can choose to have all evapotranspiration flux applied (1) as a distributed sink term, or (2) as a boundary flux (which, as in *MODPATH*, defines the evapotranspiration flux as an outflow across the top face of evapotranspiration cells, resulting in an upward velocity component on the top face of the cell). For constant-head cells that are adjacent to an aquifer boundary (or inactive cell), the user can assign the model-calculated constant-head flux to boundary faces.

FOR EACH SIMULATION, IF RECHARGE PACKAGE USED:

1. Data: IRCHTP

IRCHTP Flag to indicate how recharge is applied within cell:
0 indicates distributed source/sink term
not 0 indicates recharge is applied as a boundary flux on the top face

Notes:

If this package is not used to define IRCHTP, the model will assume $IRCHTP = 0$.

* Module is a standard *MODFLOW* input/output module.

FOR EACH SIMULATION, IF EVT PACKAGE USED:

2. Data: IEVTTP

IEVTTP Flag to indicate how evapotranspiration is applied within cell:
 0 indicates distributed sink term
 not 0 indicates evapotranspiration is applied as a boundary flux on the top face

Notes:

If this package is not used to define IEVTTP, the model will assume IEVTTP = 0.

FOR EACH SIMULATION:

3. Data: NCHNDS

NCHNDS Number of constant-head cells (defined in Basic Package by IBOUND < 0, in CHD Package, or in FHB Package as constant-head cells) for which flux is to be assigned to a boundary face, as defined in the following list in data set 4.

Notes:

For simplified input preparation in certain situations, the use of negative values will apply the boundary flux assignment to all constant-head cells within the transport subgrid, according to the following convention. If NCHNDS = -1, the source/sink flow term is distributed uniformly (per unit area) across any of the faces 1 through 4 that form boundaries with inactive cells (IBOUND = 0) or are adjacent to the external boundary of the aquifer. If NCHNDS = -2, the source/sink flow term is distributed uniformly across any of the six faces that form boundaries with inactive cells (IBOUND = 0) or are adjacent to an external boundary of the aquifer. If NCHNDS = -3, the source/sink flow term is assigned to the top face (6) of all constant-head cells located in the uppermost active layer in each row and column of the grid (that is, the uppermost active cell may lie in a different layer at various points within the grid). If NCHNDS = -4, the source/sink flow term is assigned to the bottom face (5) of all constant-head cells located in the lowermost active layer in each row and column of the grid (that is, the lowermost active cell may lie in a different layer at various points within the grid).

FOR EACH CONSTANT-HEAD CELL, IF NCHNDS > 0:

4. Data: LAYER ROW COLUMN IFACE

LAYER Layer of constant-head node.
 ROW Row of constant-head node.
 COLUMN Column of constant-head node.
 IFACE Cell face on which to assign constant-head flux.

Notes:

There must be NCHNDS lines or records in data set 4. If NCHNDS is less than or equal to 0, data set 4 is skipped. Following the convention for MODPATH (Pollock, 1994), if IFACE equals 0 or is greater than 6, the flow term is treated as an internal source or sink. If IFACE equals a number from 1 through 6, the flow term is assigned to the cell face corresponding to that value (see figure 2). (If the specified face is not a boundary face, the assignment will be ignored and the flux will remain internal to the cell.) If IFACE is less than 0, the source/sink flow term is distributed uniformly across any of the

faces 1 through 4 that form boundaries with inactive cells ($IBOUND = 0$) or are adjacent to an external boundary of the aquifer.

Concentration on Subgrid Boundary File (CBDY)

If a subgrid boundary is used in a transport simulation, the user must specify the concentration in fluid that enters the transport domain with flow across the boundary of the transport subgrid from those parts of the flow model domain that are excluded from the transport subgrid. This is normally defined in Data Set 11 of the main *GWT* input file, which allows a separate but single value to be specified for each model layer. It may be desirable, however, to allow the concentration in the fluid flux across the subgrid boundary to vary spatially. This Package allows the specification of spatially varying source concentrations to associate with (1) vertical flow across a subgrid boundary from the layer above and (or) below the transport subgrid, if the number of layers in the transport subgrid is less than the number of layers in the *MODFLOW* simulation, and (2) lateral inflow across a subgrid boundary within a *MODFLOW* layer. The data are read from a separate unit specified in the *GWT* name file for ftype "CBDY."

FOR EACH SIMULATION, IF **CBDY** PACKAGE USED:

1. Data: {CINFLA (NSCOL, NSROW)} C' to be associated with vertical fluid inflow across the upper boundary of the subgrid. Only read if ISLAY1 > 1.
Module: U2DREL*

2. Data: {CINXY (NSCOL, NSROW)}
 C' to be associated with horizontal fluid inflow across the lateral boundaries of the subgrid. Data are read for all cells; however only the cells on the boundary are used. At corner cells the user is responsible for entering an appropriate value (there can be two lateral faces at a corner; the code uses only one value for both faces). Only read if the lateral subgrid dimensions are smaller than the lateral flow grid dimensions.
Module: U2DREL*

3. Data: {CINFLB (NSCOL, NSROW)} C' to be associated with vertical fluid inflow across the lower boundary of the subgrid. Only read if ISLAY2 < NLAY, the number of layers in the *MODFLOW* grid.
Module: U2DREL*

Notes:

If this package is used, then the program will skip Data Set 11 in the main *GWT* input file. If a transport subgrid is not used, the data in this input file will not be read.

If the transport subgrid has the same row and column dimensions as the flow grid, CINXY (Record 2) should not be included in the CBDY input file.

Values are required for Records 1 and (or) 3 only if there is a flow layer above the subgrid and (or) below the subgrid, respectively. For example, Record 1 is skipped if layer 1 of the flow grid coincides with the uppermost layer of the transport subgrid (that is, ISLAY1 = 1).

Starting Stress Period File (SSTR)

MODFLOW-2000 includes the capability to simulate multiple stress periods in which some represent steady-state flow and some represent transient flow. This is commonly implemented to simulate predevelopment or natural conditions using an initial steady-state stress period, and to simulate transient conditions under modern developed (or stressed) conditions. Among other advantages, this yields an internally consistent set of heads for the start of the transient flow simulation.

Under such a simulation scenario, it may not be necessary or desired to simulate transient transport during the initial steady-state stress period for the flow simulation. When *MODFLOW* is set up to simulate multiple stress periods, this optional *GWT* Package provides the user the option to start the transport simulation in any subsequent stress period following the first one. When used, it might be common to start transport with the beginning of the second stress period. However, any stress period following the first can be specified for the initialization and start of the transport simulation.

If this Package is activated, the model will read the SSTR input file to define the stress period number in which to start the transport simulation. The data are read from a separate unit specified in the *GWT* name file for ftype "SSTR."

Because some of the input data for the transport simulation are read as auxiliary variables in the *MODFLOW* input files, and because the SSTR Package is implemented without making any changes to the *MODFLOW* input structure, the user must continue to define the solute auxiliary variables for all stress periods when auxiliary variables are read each stress period. However, the solute-related auxiliary variables defined for pre-transport stress periods will not be used or applied in the transport simulation. For example, the Well Package allows the use of "AUXILIARY CONC" to let the user define the source fluid concentration associated with an injection well. If the user indicates that an auxiliary variable is to be used, *MODFLOW* input formats require that the auxiliary variable must be used for all stress periods.

FOR EACH SIMULATION:

1. Data: IPERGWT

IPERGWT Sequential number of the *MODFLOW* stress period in which the transport simulation starts.

Notes:

IPERGWT should be ≥ 2 .

Observation Well File (OBS)

Nodes of the transport subgrid can be designated as “observation wells.” At each such node, the time, head, and concentration after each move increment will be written to a separate output file to facilitate graphical postprocessing of the calculated data. The input file for specifying observation wells is read if the file type (Ftype) “OBS” is included in the *GWT* name file.

FOR EACH SIMULATION, IF *OBS* PACKAGE USED:

1. Data: NUMOBS IOBSFL

NUMOBS Number of observation wells.

IOBSFL If IOBSFL = 0, well data are saved in NUMOBS separate files. If IOBSFL > 0, all observation well data will be written to one file, and the file name and unit number used for this file will be that of the first observation well in the list.

FOR EACH OBSERVATION WELL:

2. Data: LAYER ROW COLUMN UNIT

LAYER Layer of observation well node.

ROW Row of observation well node.

COLUMN Column of observation well node.

UNIT Unit number for output file.

Notes:

If NUMOBS > 1 and IOBSFL = 0, you must specify a unique unit number for each observation well and match those unit numbers to DATA file types and file names in the *GWT* name file. If IOBSFL > 0, you must specify a unique unit number for the first observation well and match that unit number to a DATA file type and file name in the *GWT* name file.

Particle Observation File (PTOB)

For some studies it is of interest to know not only the mean concentration in a cell, but also the statistical characteristics (such as range or variance) of the distribution of concentrations of all particles within the cell from which the mean is calculated. Nodes of the transport subgrid, or groups of nodes, can be designated as “particle observation” locations. At each such node, the cell coordinates (column, row, and layer in the main *MODFLOW* grid), total simulation time, particle concentration, and volumetric discharge rate into external sinks (two columns are reported: one with rate from standard sinks (QSINK), and one with rate from Multi-Node Wells that include nodes with both inflow and outflow (QMNWSINK)) after each move increment will be written to a separate output file to facilitate statistical postprocessing of the distribution of particle concentrations in the cell. There are also two blank columns that are reserved for use in a future release of *GWT*. The input file for specifying particle observations is read if the file type

(Ftype) “PTOB” is included in the *GWT* name file. The model distinguishes between cells comprising a Multi-Node Well (MNW) and other cells or groups of cells.

FOR EACH SIMULATION, IF *PTOB* PACKAGE USED:

1. Data: NUMPTOB NUMPTOB_MNW

NUMPTOB Number of non-MNW particle observation locations.
NUMPTOB_MNW Number of MNW particle observation locations.

FOR EACH PARTICLE OBSERVATION LOCATION DEFINED BY NUMPTOB:

2. Data: LAYER ROW COLUMN UNIT

LAYER Layer of particle observation node.
ROW Row of particle observation node.
COLUMN Column of particle observation node.
UNIT Unit number for output file.

FOR EACH PARTICLE OBSERVATION LOCATION DEFINED BY NUMPTOB_MNW:

3. Data: MNWSITE UNIT

MNWsite Name of multi-node well, as identified by using “**SITE:**” option in input data set for MNW Package (see Halford and Hanson, 2002, p. 15).
UNIT Unit number for output file.

Notes:

Unit numbers must be matched to a DATA file type and file name in the *GWT* name file. The volumetric discharge, volume removed from the particle, and mass removed from the particle account for all sinks that remove water from a cell.

If NUMPTOB > 1, the unit numbers for each particle observation location do not need to be unique; observations with the same unit number will be written to the same file and, in this way, particles associated with a group of nodes can be tracked.

If NUMPTOB_MNW > 1, the user must supply the name of a multi-node well, and each of the cells in that well will be used to record data. This file prints particle records only for cells where there is flow into the MNW (that is, the MNW is a sink in the cell). If more than one MNW is defined for a cell, the volumetric discharge will include the summed flows into each of the wells. For stress periods when the MNW is inactive, particle records will not be printed.

REFERENCES

- Goode, D.J., 1999, Age, double porosity, and simple reaction modifications for the MOC3D ground-water transport model: U.S. Geological Survey Water-Resources Investigations Report 99-4041, 34 p.
- Halford, K.J., and Hanson, R.T., 2002, MODFLOW-2000, User guide for the drawdown-limited, Multi-Node Well (MNW) Package for the U.S. Geological Survey's modular three-dimensional ground-water flow model, Versions MODFLOW-96 and MODFLOW-2000: U.S. Geological Survey Open-File Report 02-293, 33 p.
- Harbaugh, A.W., and McDonald, M.G., 1996, User's documentation for MODFLOW-96, an update to the U.S. Geological Survey modular finite-difference ground-water flow model: U.S. Geological Survey Open-File Report 96-485, 56 p.
- Heberton, C.I., Russell, T.F., Konikow, L.F. and Hornberger, G.Z., 2000, A three-dimensional finite-volume Eulerian-Lagrangian Localized Adjoint Method (ELLAM) for solute-transport modeling: U.S. Geological Survey Water-Resources Investigations Report 00-4087, 63 p.
- Hornberger, G.Z., Konikow, L.F., and Harte, P.T., 2002, Simulating horizontal-flow barriers using the MODFLOW Ground-Water Transport Process: U.S. Geological Survey Open-File Report 02-52, 28 p.
- Hsieh, P.A., and Winston, R.B., 2002, User's guide to Model Viewer, A program for three-dimensional visualization of ground-water model results: U.S. Geological Survey Open-File Report 02-106, 18 p.
- Kipp, K.L., Konikow, L.F., and Hornberger, G.Z., 1998, An implicit dispersive transport algorithm for the U.S. Geological Survey MOC3D solute-transport model: U.S. Geological Survey Water-Resources Investigations Report 98-4234, 54 p.
- Konikow, L.F., and Bredehoeft, J.D., 1978, Computer model of two-dimensional solute transport and dispersion in ground water: U.S. Geological Survey Techniques of Water-Resources Investigations, Book 7, Chapter C2, 90 p.
- Konikow, L.F., Goode, D.J., and Hornberger, G.Z., 1996, A three-dimensional method-of-characteristics solute-transport model (MOC3D): U.S. Geological Survey Water-Resources Investigations Report 96-4267, 87 p.
- Konikow, L.F., and Hornberger, G.Z., 2003, Use of boundary fluxes when simulating solute transport with the MODFLOW ground-water transport process: U.S. Geological Survey Open-File Report 03-303, 17 p.
- Konikow, L.F., and Hornberger, G.Z., 2006, Use of the Multi-Node Well (MNW) Package when simulating solute transport with the MODFLOW Ground-Water Transport Process: U.S. Geological Survey Techniques and Methods 6-A15, 34 p.
- Merritt, M.L., and Konikow, L.F., 2000, Documentation of a computer program to simulate lake-aquifer interaction using the MODFLOW ground-water flow model and the MOC3D solute-transport model: U.S. Geological Survey Water-Resources Investigations Report 00-4167, 146 p.
- Niswonger, R.G., and Prudic, D.E., 2005, Documentation of the Streamflow-Routing (SFR2) Package to include unsaturated flow beneath streams—A modification to SFR1: U.S. Geological Survey Techniques and Methods 6-A13, 48 p.
- Pollock, D.W., 1994, User's guide for MODPATH/MODPATH-PLOT, Version 3: A particle tracking post-processing package for MODFLOW, the U.S. Geological Survey finite-difference ground-water flow model: U.S. Geological Survey Open-File Report Report 94-464, 249 p.
- Prudic, D.E., Konikow, L.F., and Banta, E.R., 2004, A new streamflow-routing (SFR1) package to simulate stream-aquifer interaction with MODFLOW-2000: U.S. Geological Survey Open-File Report 2004-1042, 95 p.