DATA INPUT INSTRUCTIONS FOR GROUNDWATER TRANSPORT PROCESS (GWT)

Version (GWF1.18/GWT1.10)

The Groundwater Transport Process (GWT) is a solute-transport simulation package that is integrated with MODFLOW–2000. 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 dataset 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), Heberton and others (2000), and Konikow and Hornberger (2003). 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 (MNW2), and the Drain-Return Package. The Multi-Node Well Package Version 1 is no longer supported for solute transport. 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 groundwater 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 (MNW2) when solute transport is also simulated is described in detail by Konikow and others (2009).

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 with 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 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}.

Groundwater Transport Name File (GWT)

FOR EACH SIMULATION:

1. Data: FTYPE NUNIT FNAME

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, MOCWT, or MOCWTI 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 with the ELLAM method (as described by Heberton and others, 2000). ***MOCWT*** and ***MOCWTI*** indicate particle tracking will be done using volume-weighted particles and explicit or implicit dispersion calculation, respectively.

IPDL or IPDA Input information to describe spatially varying initial locations of particles in either list-based format (***IPDL***) or array format (***IPDA***). Only use if weighted particle method is used and ***MOCWT*** or ***MOCWTI*** are specified for the main GWT input file *[optional]*.

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]*.

PRTP 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 relative to cell dimensions. This will allow plotting packages, such as Model Viewer (Hsieh and Winston, 2002), to accurately plot relative positions 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]*.

PTOB Input file to indicate grid cells for which detailed information about particles are to be printed *[optional]*.

MBRP Separate output file with solute mass-balance components printed in a space-delimited spreadsheet. These data are printed after every transport time increment. *[optional]*.

MBIT Separate output file with solute mass-balance components as well as detailed itemization of mass transfer associated with flow packages (printed in a space-delimited spreadsheet). These data are printed after every transport time increment. *[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 Groundwater age simulation input file *[optional]*.

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 or sink fluxes (recharge, evapotranspiration, and constant-head cells) to boundary fluxes *[optional]*.

CBDY Input file to specify spatially varying source concentrations in horizontal or vertical flow across boundaries of a transport subgrid *[optional]*.

SSTR Input file to specify that transient transport calculations will begin after the first stress period of the flow simulation *[optional]*.

CCBD Constant-concentration boundary input file *[optional]*. (Not compatible with *MOC, MOCIMP*, or *ELLAM* option.)

VBAL Input file to specify list of source cells where volume balancing is to be applied *[optional]*. (Not compatible with *MOC, MOCIMP*, or *ELLAM* option.)

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 MODFLOW) can be used provided that it is not previously specified in the MODFLOW name file.

FNAME The name of the file.

Notes:

AGE, DP, and DK file types are described by Goode (1999). The CHFB file type is described by Hornberger and others (2002). The CCBD file type is described in this report.

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 and 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, MOCWT, MOCWTI*, 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, MOCIMP, MOCWT, or MOCWTI 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, although this restriction is relaxed for MOCWT and MOCWTI.

4. Data: NODISP DECAY DIFFUS

NODISP Flag for no dispersion (set NODISP=1 if no dispersion in problem; this will reduce storage allocation; in most cases, NODISP=0).

DECAY First-order decay rate [1/T] (DECAY=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, MOCIMP, MOCWT,* OR *MOCWTI* IS ACTIVE, AND *IPDL* AND *IPDA* ARE INACTIVE:

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 × NPTPND × NSROW × NSCOL × 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 0 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≤CELDIS≤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, then if *MOC* or *MOCIMP* is active, program will automatically regenerate an initial particle distribution before continuing the simulation. If the *MOCWT* or *MOCWTI* options are active and this criteria is exceeded, an attempt will be made to create a new particle on an upstream face of the cell that is void of particles with mass transferred from the upstream neighboring cell; if FZERO is still exceeded after this process, the simulation is terminated and a list of the cells with zero particles is printed to the end of the main output file. The format for this list is compatible with the input for starting locations in MODPATH (Pollock, 2012). Typically, 0.01≤FZERO≤0.10. However, to ignore this criteria for *MOCWT* or *MOCWTI* simulations (or for "debugging" model runs in which completion is more important than accuracy), specify FZERO=1.0. 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* OR *MOCWTI* IS ACTIVE:

7.1 Data: FDTMTH NCXIT IDIREC EPSSLV MAXIT

FDTMTH Weighting factor for temporal differencing of dispersion equation (0.0≤FDTMTH≤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 (NCXIT≥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.

IF *MOCWT* OR *MOCWTI* IS ACTIVE:

7.2 Data: REMCRIT GENCRIT IRAND ISRCFIX

REMCRIT REMove CRITerion for calculating minimum particle weight in a cell below which low-weight particles in (a) cells that are net fluid sinks or (b) cells adjacent to strong sources when the ISRCFIX option is used are considered to be "trivial" and are removed from the particle tracking calculations. REMCRIT represents a fraction of the volume and mass in a cell; if both the weight and mass of a particle are less than this criterion, then it is removed. Particles will not be removed if the number of particles in the cell is less than the number of particles specified in the initial distribution of particles for the cell plus 8 (that is if NPTPND(t)>(NPTPND(0)+8)). The weight and mass of the removed particle are distributed to the remaining particles in the cell. [Default value = 0.01]

GENCRIT GENerate CRITerion for determining whether a cell containing a fluid source should be considered "strong" or "weak." GENCRIT represents the fraction of the fluid flowing out of a cell that was derived from an external source; if the ratio of the net external source

flux to the total flux out of the cell is greater than this criterion, the cell is flagged as "strong." If a cell contains a strong source, new particles will be generated (created) to represent and track the source fluid. If a cell contains a weak source, the source fluid will be represented and tracked by adjusting the weights and concentrations on existing particles in the cell. If ISRCFIX=1, volume balancing will be implemented in cells where GENCRIT indicates the presence of a strong source. [Default value = 0.50]

IRAND Flag for determining method of initial positioning for newly generated particles in strong source cells. When a particle leaves a strong source, it is replaced by a new particle. If IRAND=0, the new particle is placed at the originating position of the particle that left. If IRAND>0, the particle is placed at a random location in the source cell. If IRAND=1, the "seed" value for the random number generation is itself selected randomly. If IRAND>1, the specified value of IRAND is used as the seed value.

ISRCFIX Flag for implementing volume balancing in source cells designated either by the value of GENCRIT or by listing in the VBAL Package. If ISRCFIX=0, the sum of particle weights in all source cells is allowed to change. If ISRCFIX=1, the sum of particle weights in designated source cells remains constant at the value of the fluid volume of the cell.

Notes:

Entering a 0 or out-of-range value for either of the first two variables will cause the code to use the indicated default value. Specifying the seed value by setting IRAND>1 allows the user to lock in the same sequence of "random" numbers, which may be desired when testing sensitivity of results to parameter variations.

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 ≥ 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 Konikow and others, 1996, p. 39–40). 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*, *MOCIMP*, *MOCWT*, or *MOCWTI* is active.

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

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		

[1] The Fortran formats specified here take the form rFw.d or rGw.d. For the "F" formats, the "r" represents the number of values printed per line, the "w" represents the number of characters used to represent the number and the "d" represents the number of digits in the fractional part. The "G" formats are similar except that the number of characters in the decimal part may be increased so that the number can be printed with greater precision.

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`*

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

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

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

Module: U1DREL*

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 dataset. 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

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

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 dataset 12) and in CHD or FHB, the latter values will override the former values.

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 or 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 dataset is skipped if MOCWT, MOCWTI, or ELLAM is active.

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

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. Spatially varying values of RF can be implemented as described by Goode (1999).

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

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.

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 with 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≥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*

Initial Particle Density File—List-Based Input Format (IPDL)

Input information to describe spatially varying initial locations of particles for weighted-particle method. When using weighted particles, this input approach is most applicable when the same initial particle density is desired at most cells of the grid, and either higher or lower initial particle densities are desired at just a small number of cells.

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

1. Data: NPTLAY NPTROW NPTCOL NPTLIST NPMAX

NPTLAY The number of uniformly spaced particles to be placed initially in the layer direction in each cell (except for those cells defined in part 2 of this file).

NPTROW The number of uniformly spaced particles to be placed initially in the row direction in each cell (except for those cells defined in part 2 of this file).

NPTCOL The number of uniformly spaced particles to be placed initially in the column direction in each cell (except for those cells defined in part 2 of this file).

NPTLIST The number of cells in the grid for which the density of initially placed particles will differ from the uniform default values indicated by the above three parameters. The second part of this data file must include NPTLIST lines of data.

NPMAX Maximum number of particles available for particle tracking of advective transport. If set to 0, the model will automatically calculate NPMAX according to the following equation:

$$NPMAX = 2 \times NPGRID.$$

where NPGRID is the total number of particles in all cells.

IF *NPTLIST*>0:

2. Data: LAYER ROW COLUMN NPTLAY {NPTROW NPTCOL}

LAYER Layer in which cell is located.

ROW Row in which cell is located.

COLUMN Column in which cell is located.

NPTLAY If NPTLAY is a positive number, then for this particular cell it is defined as above for Item 1. Specifying NPTLAY as a negative number indicates that the initial particles in this cell will be distributed in a radial pattern. The absolute value of NPTLAY defines how many particles are placed in the pattern and must be greater than 3. By default, the radius of the radial pattern is assumed to be 0.33 of the cell distances in the *x*- and *y*-directions. The relative *z*-coordinate is set to 0.0.

NPTROW As defined above for Item 1. Not read if NPTLAY<0.

NPTCOL As defined above for Item 1. Not read if NPTLAY<0.

Notes:

If the transport grid is only one cell wide in any direction and the number of particles specified to be placed in that direction is greater than one, then the code will automatically reduce the particle density in that direction (that is, NPTCOL, NPTROW, or NPTLAY) to a value of one.

There must be NPTLIST repetitions of Item 2. Each record will be used to specify the initial density of particles generated in the layer, row, and column directions, respectively, for that one particular cell located at the indicated (Layer,Row,Column) coordinates of the primary *MODFLOW* grid.

Initially distributing particles in a radial pattern may be useful for a cell in which a strong fluid source is located. In this case, the absolute value of NPTLAY must be greater than 3, although higher values are recommended. If the cell dimensions are equal, the pattern will be a circle. If cell dimensions are not equal, the pattern will be distorted in an elliptical shape relative to the magnitude of the dimensions.

Initial Particle Density File—Array-Based Input Format (IPDA)

Input information to describe spatially varying initial locations of particles for weighted-particle method. When using weighted particles, this input approach is most applicable when the initial particle density will vary among most cells of the grid.

1. Data: NPMAX

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

$$NPMAX = 2 \times NPGRID.$$

where NPGRID is the total number of particles in all cells.

FOR EACH LAYER OF THE TRANSPORT SUBGRID:

2. Data: NPTLAYA(NSCOL,NSROW) Initial number of weighted particles generated in layer direction.

Module: U2DINT*

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

NPTLAYA Two-dimensional array defining the number of uniformly spaced particles to be placed initially in the layer direction in each cell.

3. Data: NPTROWA(NSCOL,NSROW) Initial number of weighted particles generated in row direction.

Module: U2DINT*

NPTROWA Two-dimensional array defining the number of uniformly spaced particles to be placed initially in the row direction in each cell.

4. Data: NPTCOLA(NSCOL,NSROW) Initial number of weighted particles generated in column direction.

Module: U2DINT*

NPTCOLA Two-dimensional array defining the number of uniformly spaced particles to be placed initially in the column direction in each cell.

Notes:

If the transport grid is only one cell wide in any direction and the number of particles specified to be placed in that direction is greater than one, then the code will automatically reduce the particle density in that direction (that is, NPTCOLA, NPTROWA, or NPTLAYA) to a value of one. If any of the three parameters are to have a uniform value in a particular layer, the U2DREL array reading utility allows the specification of just a constant value for the entire array, thereby simplifying the input process (for a complete description of MODFLOW Array Reading Utilities, see Harbaugh and others, 2000, p. 86–88).

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

Volume Balancing File—List-Based Input Format (VBAL)

Input information to describe to which cells volume balancing should be applied. In general, listed cells should be fluid or solute sources. Particle tracking in these cells will be the same as if the cell was a strong fluid source.

1. Data: NBAL

NBAL The number of cells in the transport subgrid in which volume balancing should be applied. The second part of this data file must include NBAL lines of data.

2. Data: LAYER ROW COLUMN

LAYER Layer in which cell is located.

ROW Row in which cell is located.

COLUMN Column in which cell is located.

Notes:

This file is optional for use when ISRCFIX>0. The file will not be read if ISRCFIX=0.

There must be NBAL repetitions of item 2. Each record will be used to specify a particular cell where volume balancing will be implemented; such cells are located at the indicated (Layer,Row,Column) coordinates of the primary MODFLOW grid.

The volume balance will be applied in the cell for each stress period in which there is a fluid source to the cell.

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 or 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 other stress packages, BLFX uses the auxiliary variable IFACE; see "MODFLOW Source and Sink Packages" above.

FOR EACH SIMULATION, IF RECHARGE PACKAGE USED:

1. Data: IRCHTP

IRCHTP Flag to indicate how recharge is applied within cell:

0 indicates distributed source or sink term

not 0 indicates recharge is applied as a boundary flux on the top face

Note:

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

FOR EACH SIMULATION, IF EVT OR ETS 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 dataset 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 or 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 or 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 or 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 or 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 dataset 4. If NCHNDS is less than or equal to 0, dataset 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 (using MODPATH conventions). (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 or 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 dataset 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 be associated 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)} Module: U2DREL*	*C′* to be associated with vertical fluid inflow across the upper boundary of the subgrid. Only read if ISLAY1>1.
2.	Data: {CINXY(NSCOL,NSROW)} Module: U2DREL*	*C′* to be associated with horizontal fluid inflow across the lateral boundaries of the subgrid. Data are read for all cells; however, only data for 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.
3.	Data: {CINFLB(NSCOL,NSROW)} Module: U2DREL*	*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.

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.

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

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 pretransport 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.

Note:

`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.

Layer, row, and column numbers are specified for the MODFLOW grid (and not for the optional transport subgrid).

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: WELLID UNIT

WELLID Name of multi-node well, as used in input dataset 2a for MNW2 Package (see Konikow and others, 2009, p. 46).

UNIT Unit number for output file.

Notes:

Layer, row, and column numbers are specified for the MODFLOW grid (and not for the optional transport subgrid).

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 written to the output are a summation of, volume removed from the particle, and mass removed from the particle account for all sinks that remove water from the 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.

Constant-Concentration Boundary (CCBD)

This package can be used to simulate a solute-transport boundary condition in which the concentration remains constant during a stress period. For each designated constant-concentration node, the concentration value of the boundary condition must be specified. The input file for specifying CCBD cells is read if the file type (Ftype) "CCBD" is included in the GWT name file. The CCBD Package is only compatible with a volume-weighted particle option (MOCWT or MOCWTI). It is not compatible with direct-age simulations (AGE Package).

FOR EACH STRESS PERIOD, IF *CCBD* PACKAGE USED:

1. Data: ITMP

ITMP If ITMP≥0, the number of constant-concentration boundary cells this stress period.

If ITMP<0, constant-concentration boundary data from the previous stress period will be used (this option not valid for first stress period).

FOR EACH CONSTANT-CONCENTRATION BOUNDARY CELL:

2. Data: LAYER ROW COLUMN CCCONC

LAYER Layer of constant-concentration cell.

ROW Row of constant-concentration cell.

COLUMN Column of constant-concentration cell.

CCCONC Constant-concentration value that will be fixed in cell (CCCONC must be ≥0.0).

Notes:

If the initial concentration (defined in dataset 10) of a CCBD cell does not match CCCONC for that cell, the CCBD value overrides and replaces the initial concentration value specified in dataset 10. Layer, row, and column numbers are specified for the MODFLOW grid (and not for the optional transport subgrid).

If the SSTR package is used, values should only be specified for stress periods in which the solute-transport equation is being solved.

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