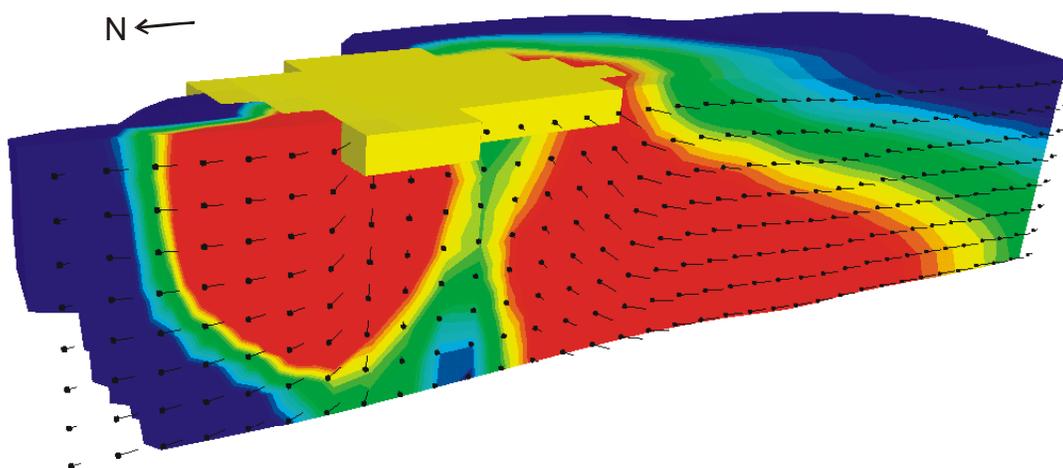




Use of Boundary Fluxes When Simulating Solute Transport With the MODFLOW Ground-Water Transport Process



U.S. GEOLOGICAL SURVEY
Open-File Report 03-303

Cover

Cropped three-dimensional visualization of solute distribution in lake-aquifer system calculated for sample problem to test BFLX Package, as described in the text of this report. Concentrations are colorized within range of 10 $\mu\text{g/L}$ (blue) to 40 or more $\mu\text{g/L}$ (red). Also shown are velocity vectors in column 16 of the grid. Lake cells are yellow.

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PREFACE

This report describes modifications to *MODFLOW-GWT*, a three-dimensional solute-transport model developed by the U.S. Geological Survey (USGS). The modifications improve the capability of *MODFLOW-GWT* to accurately simulate transport in cases that involve fluxes across the boundary of the aquifer (such as recharge at the water table). The updated *MODFLOW-GWT* model uses a new *MODFLOW* Package (BFLX) developed to implement these changes.

The code and documentation for this revised *MODFLOW-GWT* model, which includes the new BFLX Package, are available for downloading over the Internet from a USGS software repository. The repository is accessible from a Web site for USGS ground-water models at <http://water.usgs.gov/nrp/gwsoftware/> or http://water.usgs.gov/software/ground_water.html. When this code is revised or updated in the future, new versions or releases will be made available for downloading from this same site.

Although extensive testing of the modifications of the code indicates that this model will yield reliable calculations for a variety of field problems, the user is cautioned that the accuracy of the model can be affected appreciably for certain combinations of parameter values.

Use of Boundary Fluxes When Simulating Solute Transport With the MODFLOW Ground-Water Transport Process

By Leonard F. Konikow and George Z. Hornberger

ABSTRACT

This report describes modifications to a U.S. Geological Survey (USGS) three-dimensional solute-transport model (*MODFLOW-GWT*), which is incorporated into the USGS *MODFLOW* ground-water model as the Ground-Water Transport (GWT) Process. The modifications improve the capability of *MODFLOW-GWT* to accurately simulate solute transport in simulations that represent a nonzero flux across an aquifer boundary. In such situations, the new Boundary Flux Package (BFLX) will allow the user flexibility to assign the flux to specific cell faces, although that flexibility is limited for certain types of fluxes (such as recharge and evapotranspiration, which

can only be assigned to the top face if either is to be represented as a boundary flux). The approach is consistent with that used in the *MODPATH* model. The application of the BFLX Package was illustrated using a test case in which the Lake Package was active. The results using the BFLX Package showed noticeably higher magnitudes of velocity in the cells adjacent to the lake than previous results without the BFLX Package. Consequently, solute was transported slightly faster through the lake-aquifer system when the BFLX Package is active. However, the overall solute distributions did not differ greatly from simulations made without using the BFLX Package.

INTRODUCTION

Accurate simulation of solute transport depends on an accurate definition of the flow field and the accurate and precise numerical representation of velocity variations within the aquifer domain. The *MODFLOW-GWT* solute-transport model (Konikow and others, 1996; Kipp and others, 1998; Heberton and others, 2000) links several solvers for the transport equation with the *MODFLOW-2000* ground-water flow model (Harbaugh and others, 2000). Some of these solvers are based on the method of characteristics, which tracks particles moving through the active

flow field. This requires an accurate estimation of the velocity at the location of a particle, which can be at any relative location within the volume of the finite-difference cell in the grid defined for *MODFLOW*.

In *MODFLOW*, fluid sources and sinks are treated numerically as internal to a cell and as effectively distributed throughout the volume of the cell. The numerical methods used in *MODFLOW* do not distinguish between a distributed fluid source or sink and a fluid source or sink that represents a boundary flux. 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 a boundary flux, such as recharge, as a distributed source term would be consistent with having a vertical velocity of zero on the top face of the cell receiving the recharge. In the presence of recharge, however, the vertical velocity at the water-table boundary is actually nonzero. The effect of the difference between these two conceptualizations on the calculated heads is assumed to be negligible. Representing a boundary flux as a distributed source-sink term, however, affects the calculated local velocity field and advective transport, which, in turn, would affect the solution to the solute-transport equation.

MODPATH (Pollock, 1994) is a particle tracking post-processing package for *MODFLOW* that computes three-dimensional flow paths based on the cell-to-cell fluxes computed by *MODFLOW*. *MODPATH* recognizes the difference between the two alternate conceptualizations of a source/sink flux and allows the user to specify that certain fluxes represent boundary fluxes. The user can indicate which cell face the boundary flow crosses. The model then assigns that flux to the assigned face and uses it to calculate velocity. For example, recharge can 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. Whether a source/sink flux is internal to a cell or assigned to a boundary face of the cell would affect interpolation results for estimating the velocity and pathline of a particle located within a boundary cell. Thus, it would also affect concentrations calculated using *MODFLOW-GWT*.

The purpose of this report is to document the Boundary Flux Package

(BFLX), a new *MODFLOW-GWT* package that implements an option to allow assignment of fluxes to aquifer boundaries in the same manner as in *MODPATH*. This enables a more accurate and precise interpolation of velocities in finite-difference cells containing the boundary fluxes.

THEORY

Ground-water flow and velocity

The partial differential equation of ground-water flow used in *MODFLOW* is (McDonald and Harbaugh, 1988, p. 2-1):

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial h}{\partial z} \right) + W = S_s \frac{\partial h}{\partial t} \quad (1)$$

where

K_{xx} , K_{yy} , and K_{zz} are values of hydraulic conductivity along the x -, y -, and z -coordinate axes, LT^{-1} ;

h is the hydraulic (or potentiometric) head, L ;

S_s is the specific storage, L^{-1} ;

t is time, T ; and

W is the volumetric flux per unit volume representing sources and/or sinks of water, with W positive for inflow (fluid source) and negative for outflow (fluid sink), T^{-1} .

After the head distribution has been calculated for a given time step or steady-state flow condition, the specific discharge across every face of each finite-difference cell within the grid can be calculated. The specific discharge components are calculated for each face of all finite-difference cells in the grid. For example, the specific discharge (q_x) in the

horizontal plane in the x -direction at the block interface between cells (j,i,k) and $(j+1,i,k)$ is (after McDonald and Harbaugh, 1988):

$$q_{x(j+1/2,i,k)} = -\bar{K}_{xx(j+1/2,i,k)} \frac{(h_{j+1,i,k} - h_{j,i,k})}{\Delta x} \quad (2)$$

where Δx is the distance between nodes (j,i,k) and $(j+1,i,k)$, $\bar{K}_{xx(j+1/2,i,k)}$ is the interblock hydraulic conductivity in the x -direction on the forward face of the cell, and the hydraulic gradient is based on implicitly calculated heads at the adjacent nodes. Note that the interblock hydraulic conductivity is commonly defined by the harmonic mean, but in *MODFLOW* the user can specify alternative methods for calculating the interblock hydraulic conductivity.

The average interstitial velocity (V_i) (or seepage velocity) of ground water at a point can be calculated from the specific discharge as follows:

$$V_i = \frac{q_i}{\varepsilon} \quad (3)$$

where ε is the effective porosity of the porous medium (dimensionless).

When particle-tracking methods are used to represent advective transport in the algorithm to solve the solute-transport equation, the seepage velocity at any point within a cell must be defined. It may be calculated at a point of interest within a finite-difference cell based on the interpolated estimate of specific discharge at that point divided by the effective porosity of the cell in which the point is located. The *MODFLOW-GWT* model offers two interpolation schemes: linear and bilinear. However, regardless of which interpolation scheme is used, the value at the point of interest will be based on the components of specific discharge calculated on cell faces using eq. 2 and similar equations for flow in other directions.

In the case of linear interpolation, for example, each velocity component is linearly interpolated in the direction of the component of interest. The solute velocity at any particular point or location within a finite-difference cell depends on the relative distance of the point to the cell faces where the respective components of specific discharge are calculated. The linear interpolation scheme is illustrated for V_x in figure 1, which shows a particle p located in cell j,i,k . V_x at p depends on the relative position within the cell in the x -direction only, and does not vary with changes in particle position in the y - or z -directions within the cell. For this example of flow in the x -direction, δx is the spatial weight for interpolation, and is given by:

$$\delta x = \frac{x_p - x_{j-1/2,i,k}}{\Delta x} \quad (4)$$

where the subscript p indicates the particle location and δx can range from 0.0 to 1.0. V_x at p can be calculated directly from

$$V_{x(p)} = \delta x V_{x(j+1/2,i,k)} + (1 - \delta x) V_{x(j-1/2,i,k)} \quad (5)$$

More details on interpolation schemes are presented by Konikow and others (1996).

Boundary flux

Assigning an external flux to a boundary face is accomplished by using the new boundary flux input file (Ftype "BFLX") and, when appropriate, using the auxiliary parameter IFACE in list-directed sink/source packages for *MODFLOW*. These specifications will only affect transport calculations, hence are only applied within the area of the transport subgrid.

The notation used to describe cell faces and boundary flux locations is illustrated in figure 2. A three-dimensional perspective of a representative block-centered finite-

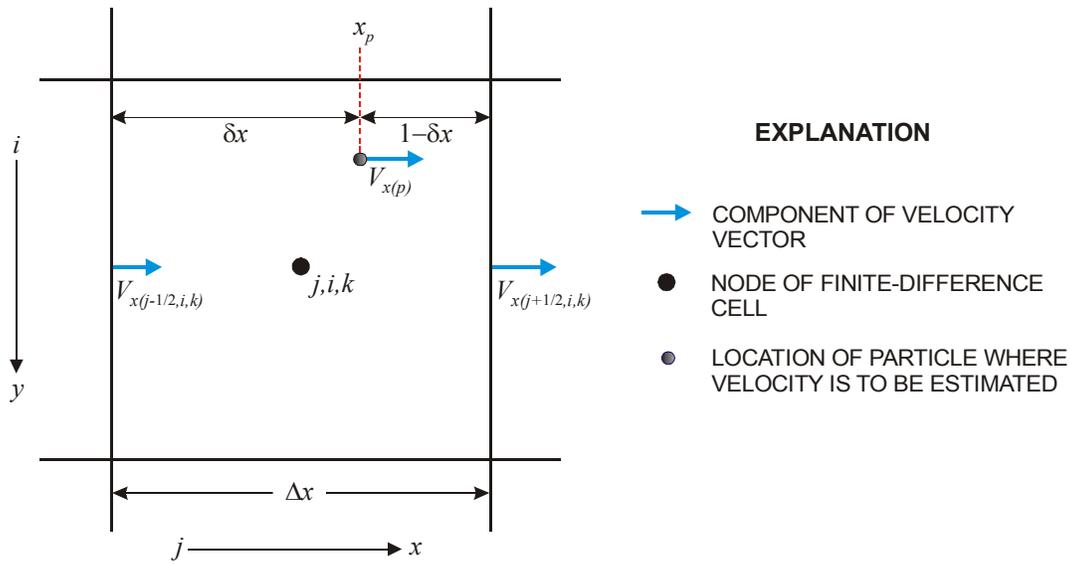


Figure 1. Plan view of representative finite-difference cell showing spatial weights used in linear interpolation method to estimate V_x at the location of a particle (modified from Konikow and others, 1996).

difference cell is depicted in figure 2A. The cell has six faces and the standard *MODFLOW* column-row-layer cell indexing notation is shown in figure 2B for reference. A stencil mapping nodal interconnections between node j, i, k (located at the center of the representative cell) and the six adjacent nodes is shown in figure 2C. Nodes are identified by their column-row-layer coordinate relative to j, i, k . This stencil also shows the arbitrary numbering system used in *MODPATH* and *MODFLOW-GWT* to identify each of the six faces located between the adjacent cells. In the code, the parameter “IFACE” stores the cell-face indicator. For example, the top face of the cell would be represented by a value of IFACE = 6, whereas the front face would have a value of IFACE = 3.

The sensitivities of interpolated velocities within a boundary cell and of calculated particle pathlines to the two alternative conceptualizations for a fluid source are demonstrated in figure 3, which shows a cross-sectional view (parallel to the front face) of a representative cell in the top

layer of a *MODFLOW* grid. In this example, the top face coincides with the aquifer boundary, and the aquifer receives recharge into the top layer. There is significant lateral flow from left to right, indicated by the velocity vectors on faces 1 and 2. There is also downward flux out of the cell across the bottom face.

Representative particle pathlines calculated for seven particles distributed vertically on the center line of the cell are shown in figure 3. If the recharge is represented as a distributed (internal) source in the cell, then the vertical flux (and velocity) on the top face would be equal to zero, and the upper aquifer boundary (the top face of this cell) would coincide with a no-flow boundary. Within the cell, the vertical velocity (V_z) increases linearly from zero on the top face to the value calculated on the bottom face. Thus, the particles located initially close to the top face of the cell move nearly horizontally (dashed arrows). On the other hand, if the recharge is applied as a boundary flux on the top surface of the cell (face 6), then the resulting particle

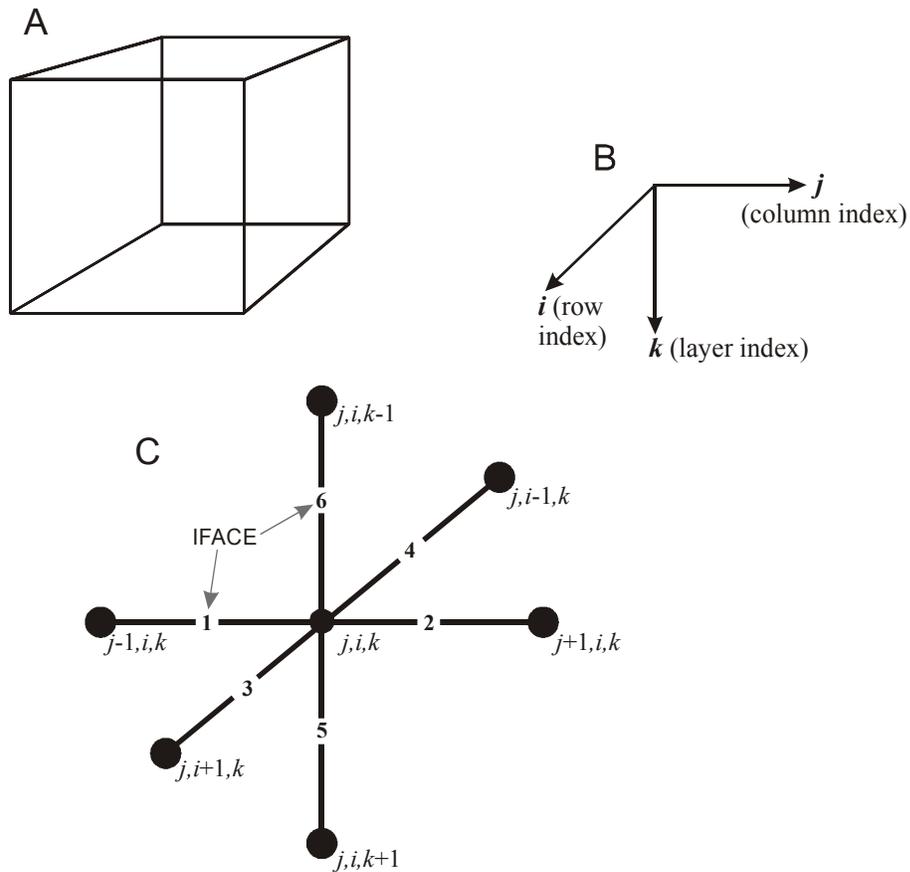


Figure 2. Schematic diagram of (A) representative cell in three-dimensional finite-difference grid; (B) notation used for column, row, and layer indexing; and (C) nodal interconnections and labeling convention for cell faces.

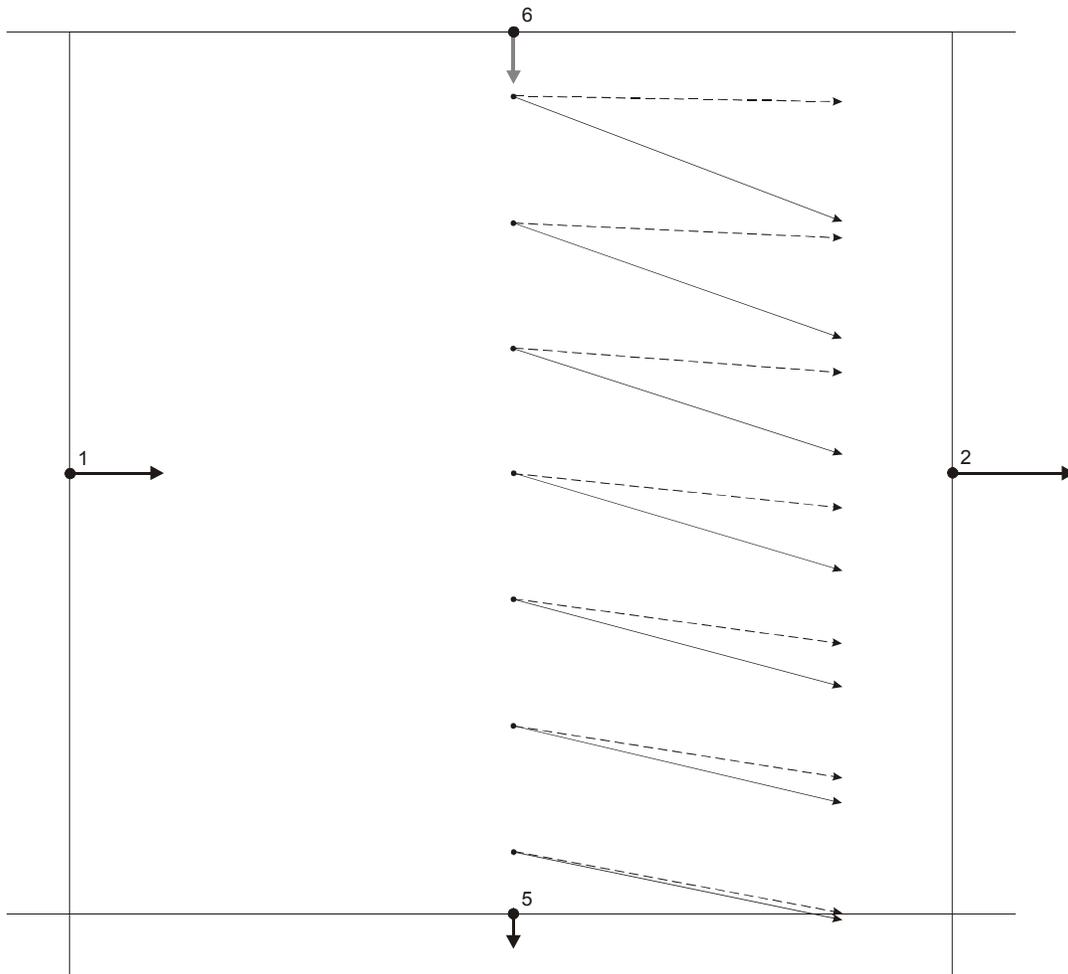
pathlines (shown as solid arrows) have a greater downward component, as would be expected for such a surficial boundary flux. The difference between the two conceptualizations diminishes as the distance from the face representing the boundary flux increases. Particle velocities in the layer below would be unaffected.

The various source/sink packages and parameters available in *MODFLOW*, along with the respective manner for specifying the flux as a boundary flux for GWT, are listed in table 1. Options to specify recharge, evapotranspiration, and constant-head (IBOUND<0) 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 designated by setting the value of IBOUND < 0,

and which are adjacent to an aquifer boundary (or inactive cell), the user can assign the model-calculated constant-head flux to a boundary face. The specified



EXPLANATION

- ⁶ IFACE value
- Velocity vector at cell face and IFACE definition (gray vector for case of boundary flux only)
- Interpolated particle pathline using boundary flux on top face
- - -→ Interpolated particle pathline with distributed flux ($V_z = 0$ on top face)

Figure 3. Effect of boundary-flux representation on calculated particle pathlines. Example shows a vertical profile parallel to the column direction through a representative cell in the top layer of a model grid.

Table 1. Boundary flux options associated with various source/sink packages in *MODFLOW*

SOURCE/SINK PACKAGE OR PARAMETER	SPECIFICATION METHOD	FACE OPTIONS
RCH	Ftype BFLX ¹	Top face only
EVT	Ftype BFLX ¹	Top face only
ETS	Ftype BFLX ¹	Top face only
WELL	AUX IFACE ²	User specified
DRAIN	AUX IFACE ²	User specified
RIVER	AUX IFACE ²	User specified
GHB	AUX IFACE ²	User specified
DRT	AUX IFACE ²	User specified
FHB (Flow cells)	AUX IFACE ²	User specified
FHB (Constant-head cells)	Ftype BFLX ¹	User specified
SFR	Implicitly assumed ³	Top face only
LAK	Implicitly assumed ³	Automatic selection
CHD	Ftype BFLX ¹	User specified
IBOUND<0	Ftype BFLX ¹	User specified

¹ See input instructions for input file for Ftype BFLX.

² When BFLX is active, use the “auxiliary” variable option within respective package to define IFACE. See *MODFLOW* input instructions (Harbaugh and others, 2000) and (or) FHB input instructions (Leake and Lilly, 1997).

³ For these packages, the source/sink flux is always assumed to represent a boundary flux when BFLX is active.

boundary face need not be limited to those on the external boundary of the grid or of the aquifer, but can also be on an internal boundary, as long as the adjacent cell is inactive.

For well, drain, river, general-head boundary (GHB), drain return (DRT), and flow and head boundary flow cells (FHB), the user can indicate that the respective flux be assigned to a boundary face by using the standard *MODFLOW* input option available in these packages to use auxiliary variables. The auxiliary variable should be named “IFACE” and the appropriate value listed where required by the input instructions. Data sets prepared with the auxiliary IFACE flag result in data files that are compatible with the GWT Process and the *MODPATH*

post-processing model. 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 fig. 2). For all cases where the user specifies the face, GWT recognizes the same option as in *MODPATH* that if IFACE is less than 0, the source/sink flow term is distributed uniformly across any of the vertical faces (1 through 4) that form boundaries with inactive cells (IBOUND=0) or the external aquifer boundary (see Pollock, 1994, p. 3-8 to 3-11). In these cases, the flux for the designated boundary condition will be apportioned among all appropriate faces on

the basis of their relative surface areas. Pollock (1994) also illustrates that well discharge can be assigned to multiple faces by listing multiple wells for the same node and assigning each part of the discharge and a separate face. Note that a face designated for boundary flux must lie adjacent to either an edge of the grid or an inactive cell.

When the Lake Package is used with *MODFLOW-GWT* and the BFLX Package is active, the model will automatically assume that fluxes occur across cell faces that represent the boundary between the lake and the aquifer. A single active aquifer cell may have more than one face adjacent to a lake—a top face or any lateral face. Similarly, when the Streamflow Routing (SFR) Package is used and the BFLX Package is active, the model will automatically assign the calculated flux to the top face of the uppermost cell underlying each stream reach. Note that there is presently (2003) no linkage available between the Ground-Water Transport Process and either the Reservoir (RES) Package or the original Streamflow Routing (STR) Packages, so these two are not listed in table 1.

COMPUTER PROGRAM AND NUMERICAL TESTS

Program design

The modifications to the *MODFLOW-GWT* code described in this report are compatible with *MODFLOW-2000* (Harbaugh and others, 2000). The GWT Process is described by Konikow and others (1996), Kipp and others (1998), and Heberton and others (2000). These modifications only are available if the GWT Process is activated. The computer coding is written in standard FORTRAN-77 and FORTRAN-90, and it has been successfully compiled and executed on multiple platforms, including Pentium-based personal computers and Unix workstations. The names and functions of subroutines added to the *MODFLOW-GWT* code to implement the BFLX Package are listed in table 2.

The new package is implemented by including the BFLX File Type in the GWT name file. Input data requirements for the BFLX Package are described in appendix A.

Table 2. *MODFLOW-GWT* subroutines for BFLX Package

Subroutine	Description
GWT1BFLX5DF	Read basic boundary flux (BFLX) data for recharge, evapotranspiration, and constant-head cells.
GWT1BFLX5AL	Allocate space for BFLX constant-head node array (NCHNDS).
GWT1BFLX5RP	Read BFLX constant-head node array (NCHNDS).
GWT1BFLX5FM	Add constant-head boundary fluxes to velocity array.
GWT1BFLX5PCK	Add source/sink package boundary fluxes to velocity array.
GWT1BFLX5LK	Add lake boundary fluxes to velocity array.

Sample problem

The new code was tested and evaluated using a variety of relevant test problems. These were used to assure that the code was working as intended, and to evaluate the sensitivity of the solution to the use of this optional package. One of these test problems is presented in more detail in this report.

This example test case simulates the migration of a sewage plume in a sand and gravel aquifer (see Merritt and Konikow, 2000, for a detailed description of this test case). The simulation uses the Lake (LAK) Package to represent shallow ponds connected to the aquifer. The system is bounded by constant-head cells along the northern and southern edges and by no-flow boundaries elsewhere. The grid includes 8

layers (each 15 ft thick), 36 rows (at equal spacing of about 406 ft), and 23 columns (at equal spacing of about 404 ft) (fig. 4). Flow is generally from north to south, as a consequence of the imposed constant-head elevations.

The model was run without the BFLX Package activated to create a basis for comparison. Then the BFLX Package was activated and the model was run again. The effect of using the BFLX Package is illustrated in a partial north-to-south cross-section along column 18 of the grid, which passes through Lake 1 (the northern lake) (see fig. 5). Velocities in the cells directly adjacent to the lake boundary are notably greater in the simulation using the BFLX Package. Nodal velocity vectors for the simulation without the BFLX Package are

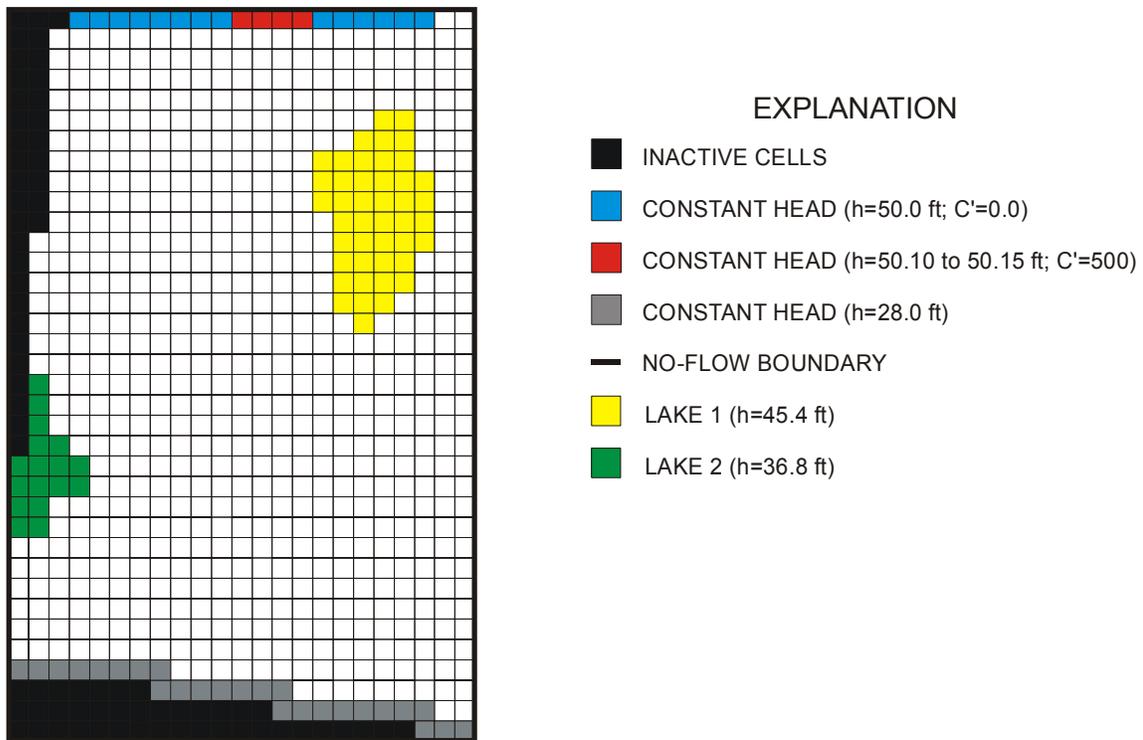


Figure 4. Areal grid and boundary conditions for sample problem with two lakes (modified from Merritt and Konikow, 2000).

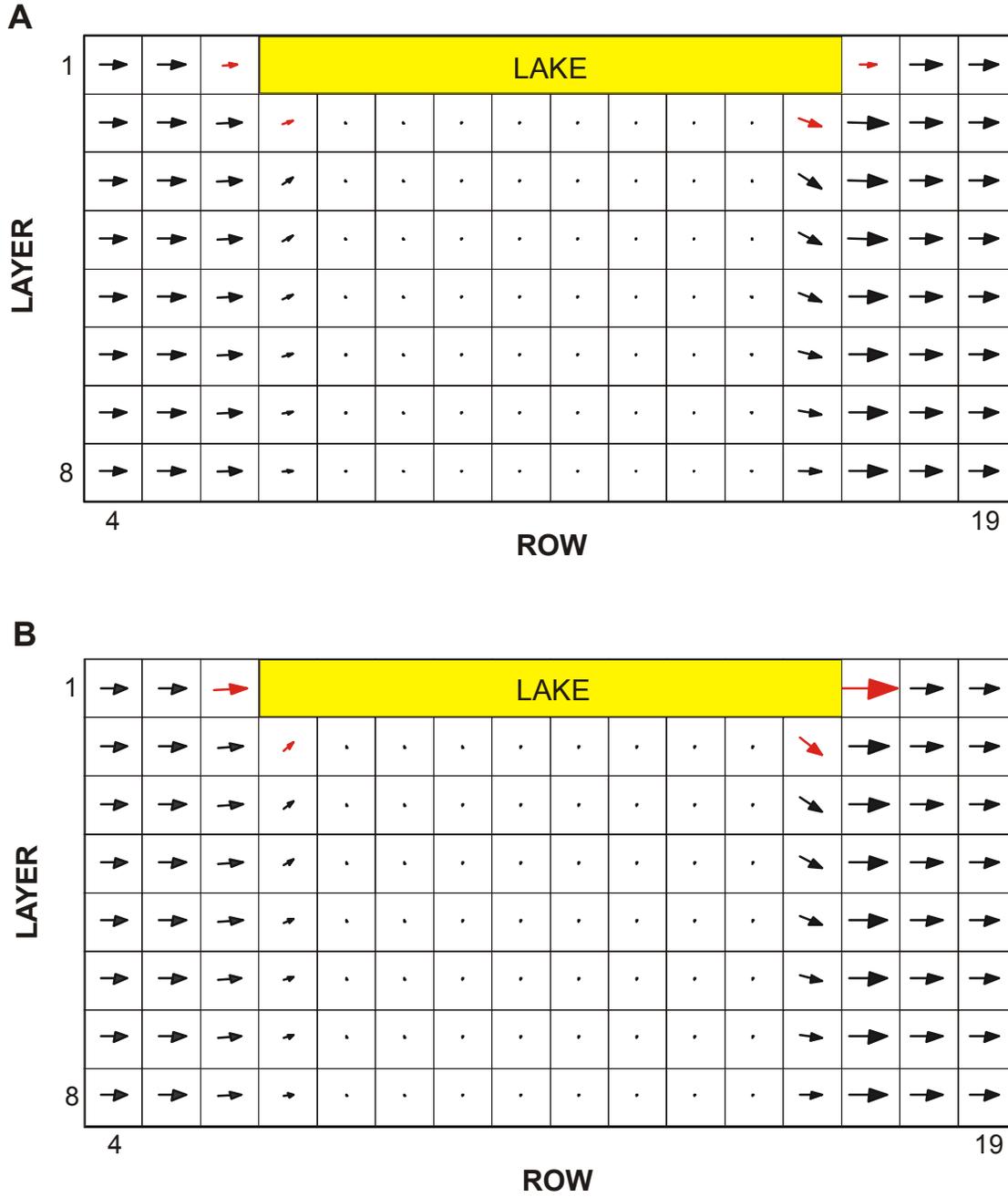


Figure 5. Partial cross section along column 18 of grid for sample problem showing nodal velocity vectors: (A) without the BLFX package, and (B) with the BLFX package active. Length and size of vector is proportional to magnitude of velocity. Vectors most affected by use of the BLFX Package are shown in red.

shown in figure 5A, and figure 5B shows results from the simulation with BFLX. In cells laterally adjacent to the lake, the horizontal components of velocity are affected, whereas in cells directly under the lake, vertical components of velocity are affected. Thus, using the BFLX Package yields higher magnitudes of velocity in cells adjacent to the lake, which would seem to more accurately represent the flow conditions near the lake in that the computed velocities would be consistent with a flux at the cell face representing the boundary between the lake and the aquifer.

Because the velocity fields differ slightly between the two simulations, the two calculated plumes are slightly different also. The calculated concentrations in layer 3 after 25 yrs for the two simulations are shown in figure 6. The differences are most evident in the contours near Lake 1. For example, the 50 and 100 $\mu\text{g/L}$ contours for the simulation without BFLX (fig. 6A) do not extend as far downgradient as the same contours for the simulation with BFLX active (fig. 6B).

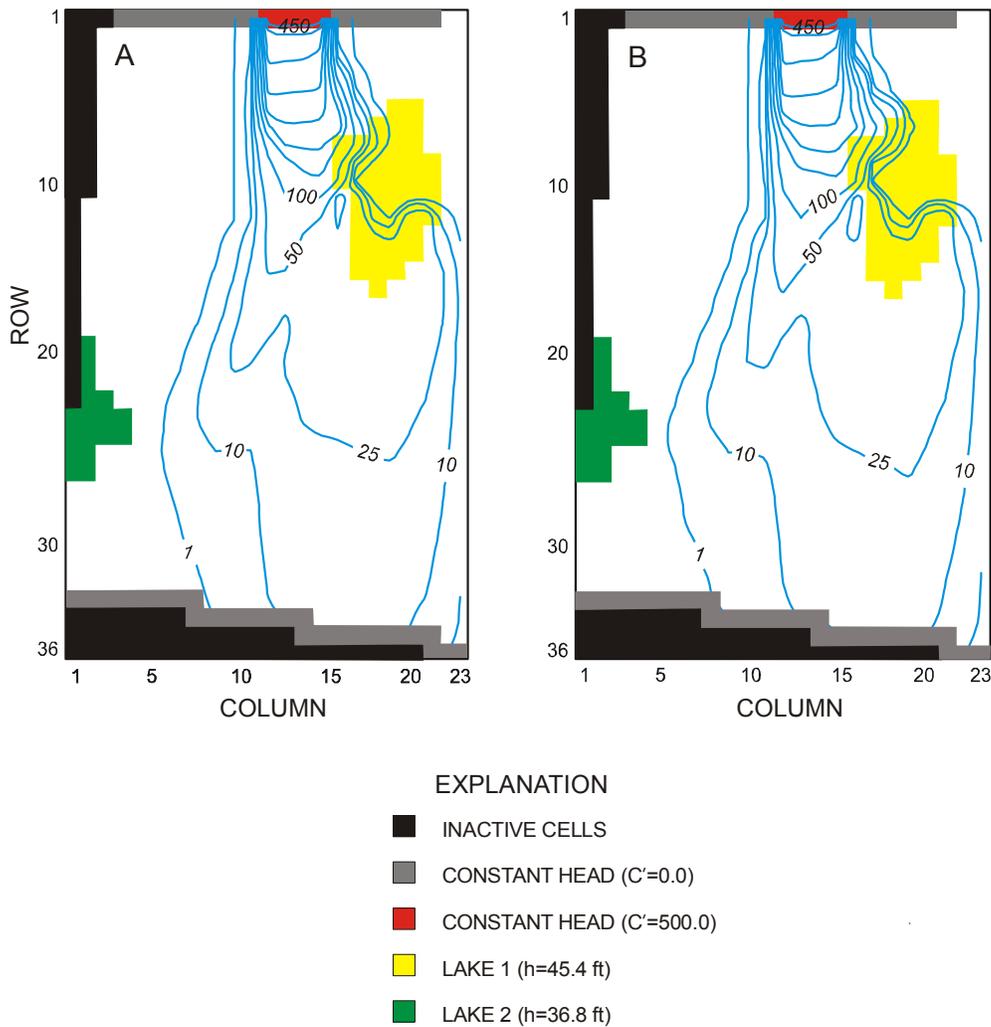


Figure 6. Maps showing calculated boron concentration (in $\mu\text{g/L}$) in model layer 3 after 25 years: (A) without the BFLX package, and (B) with the BFLX package active.

SUMMARY AND CONCLUSIONS

The Boundary Flux (BFLX) Package for the *MODFLOW-GWT* model allows the model user to specify that source/sink fluxes in boundary cells are to be considered as occurring on (or across) a boundary face rather than as an internal flux distributed uniformly throughout the volume of a cell. Because the latter and original formulation yields zero velocity on the boundary face, the new formulation will yield greater magnitudes of velocity in these boundary cells, and are consistent with a nonzero velocity on the specified cell face. This may be a more realistic condition in certain cases, such as where recharge enters the top layer of the model and a vertically downward component of velocity would be expected to occur at the water table.

The assumptions for using the BFLX Package are consistent with those used in the *MODPATH* model. However, the BFLX Package extends the boundary-flow approach to include constant-head cells, which *MODPATH* does not include. Using the BFLX Package should allow more accurate representation of velocity vectors near aquifer boundaries that are not impermeable and do not represent a “no-flow” condition. Although the related solute-transport simulation should be more accurate for such conditions, the net difference in calculated concentration fields may be quite small.

The application of the BFLX Package was illustrated using a test case in which the Lake Package was active. The results showed noticeably higher magnitudes of velocity in the cells adjacent to the lake. Consequently, solute was transported slightly faster through the lake-aquifer

system. However, the overall solute distributions did not differ greatly from simulations made without using the BFLX Package.

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APPENDIX A: DATA-INPUT INSTRUCTIONS FOR BFLX PACKAGE

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 (GWT) 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.

Ground-Water Transport Name File (GWT)

The GWT 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 (or output) file and for the main GWT input file. Following is a description of the new optional file type that can be included in the transport name file to activate the BFLX Package.

FOR EACH SIMULATION:

1. Data: FTYPE NUNIT FNAME

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 the following character string to activate BFLX:
BFLX	Input file to convert certain distributed source/sink fluxes (recharge, evapotranspiration, and constant-head cells) to boundary fluxes and to activate same conversion for other packages when using the auxiliary parameter IFACE [optional].
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 also specified elsewhere in the <i>MODFLOW</i> or <i>MODFLOW-GWT</i> name files.
FNAME	The name of the file.

Transport Boundary Flux Input File (BFLX)

The BFLX file contains options to specify recharge, evapotranspiration, and specific constant-head fluxes (including those set using the FHB or CHD Packages) as representing a

boundary flux rather than a distributed flux. The data 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.

FOR EACH SIMULATION, IF EVAPOTRANSPIRATION PACKAGE (*EVT* OR *ETS*) 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 fig. 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.

MODFLOW Source and Sink Packages

To assign a boundary flux option for a *MODFLOW* source or sink package when the BFLX Package is active, use the standard *MODFLOW* input option available in these packages to define an auxiliary variable named "IFACE." See table 1 for a list of *MODFLOW* packages that are compatible with this option. Set the $IFACE$ value for each cell in the input file for that particular package.

APPENDIX B: ANNOTATED EXAMPLES OF INPUT FILES FOR USING BFLX PACKAGE

In the data files shown below, the right side of some data lines includes a semi-colon followed by text that describes the parameters for which values are given. These comments (including the semi-colon) are not read by the program because in free format the code will only read the proper number of variables and ignore any subsequent information on that line. This style of commenting data files is optional, but users may find it helpful when viewing the content of data files.

Following (enclosed in a border) are the contents of an example BFLX input data file for a problem in which boundary flux information is defined for areal recharge and for two particular constant-head cells. Explanations are noted outside of border:

File name: *sample.bfl*

0	;	IRCHTP	← 1
2	;	NCHNDS	← 2
1 1 1 5	;	layer, row, column, IFACE	← 3
5 1 1 6	;	layer, row, column, IFACE	← 3

- ¹ Flag to indicate that recharge should be applied as a distributed source. Note: Evapotranspiration (EVT) Package not used, so IEVTTP flag not read.
- ² Number of constant-head nodes that will have a boundary flux assigned to a face
- ³ Location of constant-head node and assigned IFACE value

Following (enclosed in a border) are the contents of an example well input data file for the WELL Package for a case in which there are three wells. For both injection wells a boundary flux is assigned to the forward column face. The pumping well is defined as an internal sink. Explanations are noted outside of border:

File name: *sample.wel*

3 0	CBCALLOCATE	AUXILIARY	CONCENTRATION	AUX	IFACE	← 1
3 0						← 2
1 1 5	1.0000000000000000E-001	100.0	2			← 3
1 1 7	1.0000000000000000E-001	100.0	2			← 3
1 8 9	-2.0000000000000000E-001	0.0	0			← 3

- ¹ Number of wells, output flag, and options (including auxiliary variable IFACE, which the BFLX Package uses)
- ² Number of active wells this stress period, and output flag
- ³ Well location, stress, concentration, and IFACE value (note that an IFACE value must be given for all wells if AUX IFACE is specified as an option for the package)