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Modifications to the Lake (LAK3) Package since documented by Merritt and Konikow (2000) are listed starting from the most recent changes.

Changes to the LAK3 Package for MODFLOW-2000 version 1.19 (August 2009 and February 2010):

A bug was fixed that caused LAK3 to misread the second line in the LAK3 input file (variables THETA NSSITR SSCNCR SURFDEPTH) when the formatted read option was used.

To allow the user to better assess the reliability of the lake calculations, time-step and cumulative mass-balance errors (as percent discrepancy) are calculated for each lake and have been added to the lake budget output information in the main listing file and to the gage output file for a lake.

The Lake Package was also modified to always write IFACE values when saving data to a compact budget file. This will facilitate enhanced compatibility and consistency with MODPATH.

Variables related to the calculations of lake stage were changed to double precision. Prior to this change, differences in values for single-precision variables were causing MODFLOW to fail to converge for some simulations.

Modifications were made to the code to better evaluate the lake volume and changes to lake volume for each time step and to allow the lake to drain and fill on the basis of surface water and groundwater inflows and outflows. These modifications are:

(1) Corrections were made to the MF2K version of the Lake (LAK3) Package to simulate the connection and disconnection of two or more lakes, which originally was described in the documentation by Merritt and Konikow (2000, p. 27-30). The calculation of the adjusted lake stages for connected and disconnected lakes is done in the budget (BD) subroutine following the calculation of lake stage and groundwater interaction. The updated method for computing lake changes is the same as that in the original document except lake stages have been corrected to account for volume differences among the different connected and disconnected lakes. The method for correcting lake stages in the BD subroutine can produce inaccuracies in groundwater interaction because changes to lake stages made in BD do not account for increases or decreases in groundwater interaction with lakes during the time step in which the lake stage changed. The groundwater heads adjacent to a lake where a step change in lake stage was made in BD at the end of the previous time step will be out of balance with the new lake stage during the next time step. If the change in lake stage is large (greater than 0.5 foot or meter), the step change in the time step could result in a "wave" being developed in the groundwater that could take more than one time step to attenuate. The effect of a step change in lake stage will depend on the length of the time step, the change in lake stage, the aquifer properties, and the lakebed leakance values. Multiple adjustments to the lake stage at the end of each time step has the potential for creating a series of "waves" in the groundwater that propagate toward the lake, if the lake stage is decreased, or away from the lake, if the lake stage is increased. The inaccuracies caused by

changing lake stage at the end of the time step may be minimized by using small time steps that reduce changes in lake stage among the lakes.

(2) The calculation of a new lake stage at the end of the time step was changed to be a function of the change in lake volume during the time step. The change in lake volume over the time step is related to the volume of the lake at the beginning of the time step plus the difference in all inflows and outflows. Inflows include precipitation, runoff specified in the lake package, lake augmentation (a negative specified withdrawal rate), stream inflows, and groundwater inflow to the lake. Outflows include lake evaporation, specified withdrawal, stream outflows, and lake seepage to groundwater. The lake can drain and fill on the basis of the balance between all inflows and outflows. The mass balance of the lake is maintained by accounting for all inflows and outflows even when the lake has no water in storage (no lake stage).

(3) A fully explicit method originally documented by Merritt and Konikow (2000, p. 8) for computing groundwater interaction with lakes using the lake stage from the previous time step was added back to the program. This was done because all of the transient problems listed in the original document used the fully explicit method for computing groundwater interactions with lakes. The fully explicit method skips the Newton iteration loop used to solve lake stage during a time step. To implement a fully explicit solution of groundwater interaction with lakes, specify a THETA value between 0.0 and 0.4. The lake stage from the end of the previous time step is used to compute groundwater interaction and a new lake stage. The user is cautioned that small lake oscillations can result each time step. When a lake is connected to an outlet stream, the lake oscillations can affect groundwater interactions along the stream below the lake. Because the fully explicit method skips the Newton iteration loop, it is not recommended for simulations that include inflows from and outflows to streams.

(4) The method for computing lake stage, volume, and area had been revised in 2006 but not explained. The old method determined the relation between stage and volume on the basis of 150 stage increments and the lake volume was determined for each increment of stage. The lake volume and area could increase or decrease dramatically where the lake expanded or contracted rapidly across a layer boundary (test simulation 1 in the original document). Such an expansion or contraction of the lake area and volume over a small change in lake stage can cause numerical instabilities when the lake stage is at or very near the layer boundary (a value of 107.0 feet in test simulation 1); particularly when using a fully implicit method for solving lake stage. A function was added to smooth the transition across layer boundaries whereby the lake volume and area varies linearly when the lake stage is between two increments with differing lake areas.

(5) Variable SURFDEPTH has been added to the Lake Package to reduce numerical oscillations caused by vertical groundwater discharge across a dry lakebed or when the lake stage is nearly the same as the lakebed (less than the value of SURFDEPTH). SURFDEPTH allows the user to specify the height of small topological variations (undulations) in lake-bottom elevations that can affect groundwater discharge to lakes. SURFDEPTH decreases the lakebed conductance for vertical flow across a horizontal lakebed caused both by a groundwater head that is between the lakebed and the lakebed plus SURFDEPTH and a lake stage that is also between the lakebed and the lakebed plus SURFDEPTH. This method provides a smooth transition from a condition of no groundwater discharge to a lake, when groundwater head is below the lakebed, to a condition of increasing groundwater discharge to a lake as groundwater head becomes greater than the elevation of

the dry lakebed. The method also allows for the transition of seepage from a lake to groundwater when the lake stage decreases to the lakebed elevation. The method is similar to that implemented in the Unsaturated-Zone Flow (UZFl) Package for the GSFLOW model (Markstrom and others, 2008, p. 59-60). The original documentation for UZFl (Niswonger and others, 2006) did not include SURFDEPTH. SURFDEPTH is specified in Record 2 of the Lake Package input file, following variables THETA, NSSITR, and SSCNCR. The four variables are read using either the fixed format F10.4, I10, F10.4, F10.2, or a free format if option "FREE" has been specified in the BAS Package input file. A default value of zero is set for SURFDEPTH in the code. SURFDEPTH is read only if THETA is assigned a negative value (the negative value of THETA is then changed to a positive value internally by the code). Values of SURFDEPTH ranging from 0.01 to 0.5 have been used successfully in test simulations.

(6) Finally, the latest version of the Lake Package was tested with the original data sets and all worked the same except for test simulations 1c and 2. Test simulation 1c illustrated a lake drying and then rewetting (Merritt and Konikow, 2000, p. 24 and 25). In the original Lake Package method, no lake interaction was allowed into a dry lake from vertically or horizontally connected cells and the lake could not rewet until the average groundwater head in cells below the bottom of the lakebed was above the lakebed. The test for rewetting a lake was done in the BD subroutine where a lake would reform once the average head in all cells beneath the bottom of the lakebed was above the elevation of the lakebed. The original solution had no aquifer cells going dry, which meant that heads in layer 1 were everywhere greater than the bottom elevation of 107 feet and heads in layer 2 were everywhere greater than the bottom elevation of 97 feet (the bottom elevation of the lake). This meant that heads adjacent to the lake in layers 1 and 2 were everywhere greater than the lakebed yet no seepage from groundwater was allowed from layers 1 and 2 into the lake either vertically or horizontally. Vertical leakage from layer 2 into a lakebed in layer 1 was not allowed when the lake stage declined below 107 feet even though the heads in layer 2 beneath the lake were greater than 107 feet. In the revised formulation, vertical and horizontal seepage from layers 1 and 2 and vertical seepage from layer 3 are allowed into dry lakebed cells. Because of this change, the results of the example problem differ from those presented by Merritt and Konikow, 2000, p. 81-88). The lake did not go completely dry until the last time step of the first stress period because groundwater seepage across dry lakebed cells reduced the lake loss caused by evaporation. Also, the lake began to fill during the first time step of the second stress period because inflow from precipitation and groundwater exceeded lake evaporation. The lake in problem 1C dries much quicker if the evaporation rate is changed from 0.0412 in the original problem to 0.0452.

Test simulation 2 illustrated how lakes can have surface inflow from streams and lake discharge to an outlet stream. Lake stages in lakes 1 and 2 in the test simulation are 1.07 and 1.25 ft less, respectively, using code modified since 2006 from that presented by Merritt and Konikow (2000, p. 25-27 and p. 89-107). The reason for these discrepancies is a difference in how outflow from a lake into a stream is computed between the original version and versions since 2006. Test simulation 2 specified the ICALC1 option in the Streamflow Routing Package (Prudic and others, 2004). This option uses Mannings equation and assumes steady uniform flow in a wide rectangular channel. The calculation of flow in a wide rectangular channel is not multiplied by two thirds as listed by Merritt and Konikow (2000, equation 11, p. 11). Thus, the lake stage and lake volume is overestimated in the original document even though the lake outflows computed in the original document are similar to those in the revised computer

code since 2006. The higher simulated lake stages also resulted in slightly higher groundwater heads near the two lakes.

LAK3 Package updates (May-July 2006) for MODFLOW-2000 and LAK7 Package updates for MODFLOW-2005: Modifications by D.E. Prudic and R.G. Niswonger

An important change was made in the computation of lake stage for steady state and transient simulations as described in the documentation report for the Lake (LAK3) Package (Merritt and Konikow, 2000). The Newton iteration loop used to calculate the steady-state lake stage (equation 12 in Merritt and Konikow, p. 12) was revised to include the calculation of outflow from a lake to streams and its derivative with respect to lake stage. Previously, lake outflow and its derivative were computed in the Streamflow-Routing (SFR1 or SFR2) Package, which did not allow the outflow and its derivative to change as the lake stage changed in the Newton iteration within the Lake Package (Prudic and others, 2004 and Niswonger and Prudic, 2005). The Streamflow-Routing Package (SFR2) also was modified to be compatible with these most recent changes in the Lake Package.

The Lake Package did not iterate internally to calculate lake stage during transient simulations. The original method of calculating transient lake stages was based on equation 10 of Merritt and Konikow (2000, p. 9), which relied on the lake outflow from the previous MODFLOW iteration. This approach resulted in non-convergences in ground-water head during transient simulations caused by oscillations in lake stage and lake outflow to streams. This problem did not necessarily cause non-convergence in ground-water cells connected to lake cells. Rather, oscillations in outflow from a lake could cause non-convergence in MODFLOW cells that interacted with stream reaches downstream of the lake outflow. To fix this problem, the computation of lake stage for transient simulations was changed to solve for lake stage using equation 12 of Merritt and Konikow (2000, p.9) such that lake outflow to streams and its derivative are now calculated within the Lake(LAK3)Package Formulate Module during transient simulations.

Although the data input structure was not altered, the new method of solving for lake stage uses only the time-weighting factor THETA (Merritt and Konikow, 2000, p. 52) for transient simulations. THETA is automatically set to a value of 1.0 for all steady-state stress periods. THETA for transient simulations has been revised and is now limited to range from 0.5 to 1.0. A value of 0.5 represents the stage midway between the previous time step and the end of the current time step. A value of 1.0 (fully implicit) represents the lake stage at the end of the current time step. A THETA of less than 0.5 does not perform well and a zero value is undefined in the Newton iteration method. Slight errors in the solution of lake stage and seepage may result when THETA is greater than 0.5 (Fread, 1993). Fread recommended a value greater than 0.5 for damping oscillations in streamflow-routing equations. A value of 0.5 represents a semi-implicit method that is often called Crank-Nicolson (Wang and Anderson, 1982, p. 81). Wang and Anderson present results for drawdown for a simple confined aquifer with pumping in which the Crank-Nicolson method produced the best results when compared with the Theis solution for different times. A value of 0.5 is generally recommended.

Test simulation 1 presented by Merritt and Konikow (2000, p. 21-23) was used to test different values of THETA for a transient simulation using the original method of computing lake stage and the revised method. Three simulations were done using the original method (THETA=0.0, 0.5, and 1.0). ATHETA of 0.5 produced changes in lake stage and ground inflow and outflow that

were midway between those computed using THETA of 0.0 and 1.0. The maximum difference in lake stage from that computed using a THETA of 0.5 was 0.324 feet at time steps 38 and 39. The percent difference with respect to the total lake stage was 0.25 percent. The maximum difference in lake inflow was 3,400 cubic feet per day at time steps 21 and 22 or 2.3 percent different than the lake inflow when THETA was 0.5. The greatest percent difference was 2.66 percent at time step 57.

Two simulations were done using the new method of iterating on lake stage during a MODFLOW iteration using the Newton method. The results for THETA = 0.5 and 1.0 were identical to those of the original method. All solutions resulted in the same lake stage and lake inflow at the end of the simulation. A THETA of 1.0 decreased the number of Newton iterations. However, the total number of MODFLOW iterations increased.

If the model simulation includes a steady-state stress period, then the number of iterations (NSSITER) and the closure tolerance (SSCNCR) defined by Merritt and Konikow (2000, p. 52) for ending the Newton iteration method is used for all subsequent transient or steady-state stress periods. If the model simulation only includes transient stress periods, a default value of 0.0001 is assigned to SSCNCR and a default value of 100 is assigned to NSSITR. An option was created in which values of SSCNCR and NSSITR can be read for a transient only simulation by placing a negative sign immediately in front of THETA. A negative THETA sets a flag which assumes input values for NSSITR and SSCNCR will follow THETA in the format as described by Merritt and Konikow (p. 52). A negative THETA is automatically reset to a positive value after values of NSSITR and SSCNCR are read.

The revised Newton method may not always find a solution to the lake stage because of discontinuities among lake stage, area, and outflow. This is particularly so for steady-state simulations of lakes with stream outflow. A warning statement is printed whenever the Newton method cannot find a solution within NSSITR iterations for the stage of a particular lake. The printed warning statement also lists the last two lake stages prior to ending the Newton iteration loop in the Formulate Module of the Lake Package.

The results using the new solution method may differ from the results using the old method. The differences will be most evident for previous simulations that have lake outflow to one or more streams or when a fully explicit time weighting (THETA = 0.0) was used for transient simulations. Differences in results of transient simulations when THETA was fully explicit will be dependent on the time steps used in the simulation.

The water budget of each lake also was revised to continue accounting for all inflows and outflows while a lake is dry. The method of filling a dry lake was also changed. All surface water inflows to a lake are summed prior to computing lake seepage losses and outflow from a lake to one or more streams. The inflow volume of a dry lake is first checked against the specified withdrawals and then against lake evaporation. If the combination of these values exceeds inflow they are reduced to equal the surface inflow. Any excess surface inflow is then available to limit the seepage from the lake to ground water. Ground-water seepage to the lake is added to surface inflow each Newton iteration and compared with the specified lake evaporation rate. If the revised total inflow exceeds the specified evaporation rate times the area of the lowest elevation of the lake bottom, then the lake is allowed to fill on the basis of the lakebed conductance values and the difference in head between lake and groundwater. The rate of filling of a dry lake will be dependent on the

elevation of the outlet elevation of the stream or streams. A stream outlet cannot be less than the lowest elevation of the lake otherwise the Newton method will not solve properly.

Modifications to the Lake (LAK3) Package by L.F. Konikow (February 2006):

Several minor coding changes were made during the past year to fix bugs and improve allocation accuracy. This required that the unit number for the GAGE Package be passed into the LAK3 allocation subroutine when called from main. Also, LSKLK and LSDONE are now allocated space in the IR array rather than into the RX array. A bug in the LAK3 budget subroutine was fixed (previously, in cases in which a lake that had gone dry was underlain by a confined type of layer, an undefined variable caused a run-time error).

Modifications to the Lake (LAK3) Package by M.L. Merritt and L.F. Konikow (Oct. 2003 and Jan. 2004):

The Lake Package has been modified to enable it to run with (1) mixed steady-state and transient stress periods, and (2) the top layer being a confined layer. Neither of these conditions was previously allowed in a simulation using the Lake Package.

(1) For mixed steady-state/transient runs, NSSITR and SSCNCR must be defined in Record 2 in the input file for the Lake Package, even if the steady-state stress period is not the first one. If more than one steady-state stress period is included in the total simulation period, then the initial values of NSSITR and SSCNCR will apply to all subsequent steady-state stress periods. If NSSITR and SSCNCR are needed and read in as a value of zero, then default values of NSSITR = 50 and SSCNCR = 0.01 will automatically override the zero values.

The capability for using mixed steady-state/transient runs with the Lake Package does not depend on the sequence of steady-state and transient stress periods. Input of minimum and maximum lake stages is as before (in Record 3) if the first stress period is steady-state (this assures compatibility with older data sets). If the second or a subsequent stress period is steady-state, then the minimum and maximum stages (SSMN and SSMX) for those stress periods are defined at the end of Record 9a. With this new option, the definition for Record 9a on p. 55 of Merritt and Konikow (2000) is modified to:

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Record 9a. Data: PRCPLK EVAPLK RNF WTHDRW {SSMN} {SSMX}
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where SSMN and SSMX are optional parameters that are only defined for a steady-state stress period that is not the first stress period in the simulation.

(2) The Lake package can now be used when all or some of the model layers containing the lake are confined. We recommend using the Layer-Property Flow Package (LPF) for this case, although the BCF and HUF Packages will work too. However, when using the BCF6 package to define aquifer properties, lake/aquifer conductance values in the lateral direction are based solely on the lakebed leakance (and not on the lateral transmissivity of the aquifer layer). As before, when the BCF6 package is used, vertical lake/aquifer conductance values are based on lakebed conductance and on the vertical hydraulic conductivity of the aquifer layer underlying the lake when the wet/dry option is implemented, and only on the lakebed leakance when the wet/dry option is not implemented.

(3) Other minor changes to output formats have been made.

(4) Because the Lake Stage represents a hydraulic head value that is consistent with the calculated heads in the aquifer, the calculated values of lake stage will now be inserted into the HNEW array at the appropriate locations. This will enable contouring or visualization of heads based on hydraulic continuity between the aquifer and a lake. Previously, because lake cells correspond with values of IBOUND=0, the HNEW array contained values of HNOFLO at lake cells. If drawdown is printed, the drawdown values shown for lake cells will represent the initial lake stage rather than HNOFLO values (as in earlier versions of the code).

(5) The Lake Package now checks for consistency between lake cell locations and values of IBOUND, which are supposed to be 0 at lake cells. If the code detects a lake cell where the value of IBOUND is not = 0, it will print a warning message (but execution will continue).

(6) A bug was corrected to assure that a lake cell can occur in the bottom layer of the grid. Previously, if the executable code had been generated with certain compilers, an array bounds error would occur in this situation.

#### References:

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Merritt, M.L., and Konikow, L.F., 2000, Documentation of a computer program to simulate lake-aquifer interaction using the MODFLOW ground-water model and the MOC3D solute-transport model: U.S. Geological Survey Water Resources-Investigations Report 00-4167, 146 p.

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