**Please open the COMUS code using Visual Studio.**

To ensure a fair comparison with MODFLOW-2005 and MODFLOW-NWT, we save the output results of COMUS-PAAC in binary format and track the computation time. Additionally, for expert review convenience, we have also provided the COMUS-PACC program that saves the results in a readable TXT file format. The source code for both programs has been attached.

**Input and output document**

**Input data**

**1 CtrlPar.in file**

The CtrlPar.in file contains the control parameters used in the simulation.

**NUMLYR**- is the number of layers in the model grid.

**NUMROW**- is the number of rows in the model grid.

**NUMCOL**- is the number of columns in the model grid.

**DIMUNIT**- is the length unit of model data (L).

**TIMEUNIT**- is the time unit of model data (T).

**XSTCORD**- is the X-coordinate at the upper-left corner of the model grid (L).

**YSTCORD**- is the Y-coordinate at the upper-left corner of the model grid (L).

**SIMMTHD**-is the simulation method option code.

1-the Picard iteration-based Always active cell (PAAC) method was selected for the simulation.

2-the MODFLOW-2005 method was selected for the simulation.

**SIMTYPE**-is the steady state/transient option code.

1-the simulation is steady state.

2-the simulation is transient.

**LAMBDA-** is the user-specified retardation factor bewteen 0.0001 and 0.001 for the steady-state finite difference flow equation of drying resistant cells. This variable is read only if SIMMTHD=1 and SIMTYPE=1.

**-**1-this option is not active.

**ISOLVE**-is the solver option code

1-Strongly-Implicit Procedure (SIP).

2-Preconditioned Conjugate Gradient (PCG).

**MAXIT**-is the user-specified maximum number of outer iterations.

**DAMP**-is the user-specified global relaxation factor between 0.0 and 1.0.

**HCOLSE**-is the head change criterion for convergence (L).

**RCLOSE**-is flux change criterion for convergence (L3/T).

**IRELAX**-is the cell-by-cell relaxation mechanism option code

0-the cell-by-cell relaxation mechanism is inactive.

1-the cell-by-cell relaxation mechanism is active.

**THETA**-is the decreasing factor of the adaptive relaxation factors, this variable is read only if IRELAX=1.

**GAMMA**-is the increasing factor of the adaptive relaxation factors, this variable is read only if IRELAX=1.

**AKAPPA**-is the single-step increase value of the adaptive relaxation factors, this variable is read only if IRELAX=1.

**NITER**-is the iteration inteval for attempting to increase the adaptive relaxation factor, this variable is read only if IRELAX=1.

**HNOFLO**- is the value of head (L) to be assigned to all no-flow cells, inactive cells and dry cells.

**ICHFLG**-indicates whether the flow between adjacent constant-head cells should be calculated.

0-no.

1-yes.

**IWDFLG**-is the Cell drying and rewetting option code

0-cell drying is active and cell rewetting is inactive, this variable is read only if SIMMTHD=2.

1-the trial-and-error method employed by MODFLOW-2005 and other earlier MODFLOW versions was used to simulate the drying-rewetting problems, this variable is read only if SIMMTHD=2.

**WETFCT**-is a factor that is included in the calculation of the head that is initially established at a cell when the cell is converted from dry to wet, this variable is read only if SIMMTHD=2 and IWDFLG=1.

**NWETIT**-is the iteration interval for attempting to wet cells, this variable is read only if SIMMTHD=2 and IWDFLG=1.

**IHDWET**- is a flag that determines which equation is used to define the initial head at cells that become wet, this variable is read only if SIMMTHD=2 and and IWDFLG=1.

0-this equation is used:

1- this equation is used:

**IMULTD**- is the parallel computing option code

0-the parallel computing is inactive.

1-the parallel computing is active.

**NUMTD**-is the number of threads used for parallel computing.

**2 Discrete.in file**

Discretization information is read from the Discrete.in file

**ATTI**

If ATTI =R, means the DELT is the cell width along rows.

If ATTI =C, means the DELT is the cell width along columns.

**NUMID**-is the row or column number.

**DELT**-is the cell width along rows or columns (L).

**3 Layer.in file**

Input for the Layer-Property Flow(LPF) is read from the Layer.in file.

**LYRID**-is the layer number.

**LYRTYPE**-contains a flag for each layer that specifies the layer type.

0-confined.

1-convertible.

**LYRHANI**-contains a value for each layer that is a flag or the horizontal anisotropy.

-1-indicates variable HANI (in Cell.in file) defines horizontal anisotropy.

>0-indicates LYRHANI is the horizontal anisotropy for the entire layer, and HANI is not read (in Cell.in file).

**LYRVKA**-contains a flag for each layer that indicates whether variable VKA (in Cell.in file) is vertical hydraulic conductivity or the ratio of horizontal to vertical hydraulic conductivity.

0-indicates VKA is vertical hydraulic conductivity

1-indicates VKA is the ratio of horizontal to vertical hydraulic conductivity, where the horizontal hydraulic conductivity is specified as HK in cell.in file.

**LYRCBD**-Quasi–3D confining bed flag.

0-there is no Quasi–3D confining bed below the layer.

1-there is a Quasi–3D confining bed below the layer.

**4 Cell.in file**

The Cell.in file contains the hydraulic parameters of model cells.

**ILYR**-is the layer number of cells.

**IROW**- is the row number of cells.

**ICOL**- is the column number of cells.

**CELLTOP**-is the top elevation of cells (L).

**CELLBOT**- is the bottom elevation of cells (L).

**IBOUND**-contains a code for each cell that indicates whether the head varies with time.

-1-means constant-head cell.

0-means no flow or inactive cell.

1-means variable-head cell.

**HK**-is the horizontal hydraulic conductivity along rows (L/T),

**HANI**- Ratio of horizontal hydraulic conductivity along columns to hydraulic conductivity along rows, this variable is read only if LYRHANI=-1.

**VKA**-Vertical hydraulic conductivity (L/T) or the ratio of horizontal hydraulic conductivity along rows (HK) to vertical hydraulic conductivity (depend on LYRVKA).

**VKCB**-is the vertical hydraulic conductivity (L/T) of a confining bed below a layer, this variable is read only if LYRCBD=1.

**TKCB**-is the thickness (L) of a confining bed below a layer, this variable is read only if LYRCBD=1.

**SC1**-is the specific storage of cells (1/L).

**SC2**-is the specific yield of cells.

**WETDRY**- is the wetting threshold (L) combined with a wetting flag for the trial-and-error method employed by MODFLOW-2005 and other earlier MODFLOW versions, this variable is read only if SIMMTHD=2 and IWDFLG=1.

<0- indicate that wetting is based only on the head in the dry cell below.

=0- indicate that deactivates wetting for the dry cell.

>0- indicate that wetting is based on head from the four surrounding horizontal cells and the cell below.

**SHEAD**-is the initial head of cells (L).

**5 Period.in file**

Information for stress periods is read from the Period.in file.

**IPER**- is the stress period number.

**PERLEN**- is the length of a stress period (T).

**NSTEP**- is the number of time steps into which a stress period is to be divided.

**MULTR**- is the time step multiplier. The time step multiplier is the ratio of the length of each time step to that of the preceding time step.

**6 BndOpt.in File**

The BndOpt.in File contains the names of boundary conditions used in this paper and controls whether or not a boundary is active.

If **SIMRCH**=1, then the Recharge Package is active. If SIMRCH=0 then the Recharge Package is inactive.

If **SIMGHB**=1, then the General-Head Boundary Package is active. If SIMGHB=0 then the General-Head Boundary is inactive.

If **SIMWEL**=1, then the Well Package is active. If SIMWEL=0 then the Well Package is inactive.

If **SIMDRN**=1, then the Drain Package is active. If SIMDRN=0 then the Drain Package is inactive.

**7 Rch.in file**

Input to the Recharge Package is read from the Rch.in file.

**IPER**- is the stress period number.

**ILYR**-is the layer number of cells

**IROW**- is the row number of cells

**ICOL**- is the column number of cells

**IRECH**-is the recharge option code

1-Recharge is applied to the specified layer in each vertical column.

2-Recharge is applied to the highest active cell in each vertical column.

**RECHR**-is the recharge flux (L/T).

**8 Ghb.in file**

Input to the General-Head Boundary Package is read from the Ghb.in file.

**IPER**-is the stress period number.

**ILYR**-is the layer number of the cell affected by the head-dependent boundary.

**IROW**-is the row number of the cell affected by the head-dependent boundary.

**ICOL**-is the column number of the cell affected by the head-dependent boundary.

**SHEAD**-is the boundary head at the start of the stress period (L).

**EHEAD**-is the boundary head at the end of the stress period (L).

**COND**-is the hydraulic conductance of the interface between the aquifer cell and the boundary (L2/T).

**9 Well.in file**

Input to the Well Package is read from the Well.in file.

IPER- is the stress period number.

ILYR- is the layer number of the cell that contains the well.

IROW- is the row number of the cell that contains the well.

ICOL- is the column number of the cell that contains the well.

WELLR-is the volumetric recharge rate (L3/T). A positive value indicates recharge and a negative value indicates discharge (pumping).

SATTHR-is the user-specified saturated thickness threshold of the well cell. The pumping rate decrease as the head drops below SATTHR.

**10 Drn.in file**

Input to the Drain Package is read from the Drn.in file.

**IPER**-is the stress period number.

**ILYR**-is the layer number of the cell containing the drain

**IROW**-is the row number of the cell containing the drain

**ICOL**-is the column number of the cell containing the drain

**DLEVE**-is the bottom elevation of the drain (L).

**COND**-is the hydraulic conductance of the interface between the aquifer and the drain (L2/T).

**11 OutOpt.in file**

Input to the Output Control Option is read from the OutOpt.in file.

**GDWBDPRN**-is the output flag for overall volumetric budget printout.

0-data is not printed.

1- data is printed for each time step of each period.

2- data is printed for each stress period.

**LYRBDPRN**-is the output flag for layer-by-layer volumetric budget printout.

0-data is not printed.

1- data is printed for each time step of each period.

2- data is printed for each stress period.

**CELLBDPRN**- is the output flag for cell-by-cell volumetric budget printout.

0-data is not printed.

1- data is printed for each time step of each period.

2- data is printed for each stress period.

**CELLHHPRN**- is the output flag for head printout.

0-data is not printed.

1- data is printed for each time step of each period.

2- data is printed for each stress period.

**CELLDDPRN**- is the output flag for drawdown printout.

0-data is not printed.

1- data is printed for each time step of each period.

2- data is printed for each stress period.

**CELLFLPRN**-is the output flag for cell-by-cell volumetric flow printout.

0-data is not printed.

1- data is printed for each time step of each period.

2- data is printed for each stress period.

**Output data**

**1 GWBD.out file**

Overall volumetric budget values are saved in GWBD.out file.

**IPER**- is the stress period number.

**ISTEP**- is the time step number of a stress period, this variable is valid only if GDWBDPRN=1.

**TLEN**- is the total simulation time.

**STAIN**-is the cumulative flow volume from storage from the beginning of the simulation (L3).

**RCHIN**-is the cumulative recharge inflow volume from the beginning of the simulation (L3) .

**GHBIN**-is the cumulative general-head inflow volume from the beginning of the simulation (L3).

**WELIN**-is the cumulative well inflow volume from the beginning of the simulation (L3).

**DRNIN**- is the cumulative drain inflow volume from the beginning of the simulation (L3).

**CNHIN**-is the cumulative constant-head inflow volume from the beginning of the simulation (L3).

**STAOUT**-is the cumulative flow volume to storage from the beginning of the simulation (L3).

**RCHOUT**-is the cumulative recharge outflow volume from the beginning of the simulation (L3).

**GHBOUT**-is the cumulative general-head outflow volume from the beginning of the simulation (L3).

**WELOUT**-is the cumulative well outflow volume from the beginning of the simulation (L3).

**DRNOUT**- is the cumulative drain outflow volume from the beginning of the simulation (L3).

**CNHOUT**-is the cumulative constant-head outflow volume from the beginning of the simulation (L3).

**ABER**-is the cumulative budget error (L3) .

**RBER**-is the total percentage budget error (%).

**2 LyrBD.out file**

Layer-by-layer volumetric budget values are saved in LyrBD.out file.

**IPER**- is the stress period number.

**ISTEP**- is the time step number of a stress period, this variable is valid only if LYRBDPRN=1.

**TLEN**- is the total simulation time (T, depend on LYRBDPRN).

**ILYR**- is the layer number.

**TOPIN**-is the cumulative leakage volume from the upper aquifer layer from the beginning of the simulation (L3).

**BOTIN**-is the cumulative leakage volume from the underlying aquifer layer from the beginning of the simulation (L3).

**RCHIN**-is the cumulative recharge inflow volume from the beginning of the simulation (L3).

**GHBIN**-is the cumulative general-head inflow volume from the beginning of the simulation (L3).

**WELIN**-is the cumulative well inflow volume from the beginning of the simulation (L3).

**DRNIN**- is the cumulative drain inflow volume from the beginning of the simulation (L3).

**CNHIN**-is the cumulative constant-head inflow volume from the beginning of the simulation (L3).

**TOPOUT**- is the cumulative leakage volume to the upper aquifer layer from the beginning of the simulation (L3).

**BOTOUT**- is the cumulative leakage volume to the underlying aquifer layer from the beginning of the simulation (L3).

**RCHOUT**-is the cumulative recharge outflow volume from the beginning of the simulation (L3).

**GHBOUT**-is the cumulative general-head outflow volume from the beginning of the simulation (L3).

**WELOUT**-is the cumulative well outflow volume from the beginning of the simulation (L3).

**DRNOUT**- is the cumulative drain outflow volume from the beginning of the simulation (L3).

**CNHOUT**-is the cumulative constant-head outflow volume from the beginning of the simulation (L3).

**ABER**-is the cumulative budget error (L3).

**3 CellBD.out file**

Cell-by-cell volumetric budget values are saved in CellBD.out file.

**IPER**-is the stress period number.

**ISTEP**-is the time step number of a stress period, this variable is valid only if CELLBDPRN=1.

**DLEN**- is the time span during current time step or stress period (T, depend on CELLBDPRN).

**ILYR**-is the layer number of cells

**IROW**- is the row number of cells

**ICOL**- is the column number of cells

**FBC**-is the net flow volume from the six adjacent cells during the time step or the stress period (L3, depend on CELLBDPRN). A positive value indicates that the net flow is into the cell and a negative value indicates that the net flow is away from the cell.

**RCH**-is the net recharge flow volume during the time step or the stress period (L3, depend on CELLBDPRN). A positive value indicates that the net flow is into the cell and a negative value indicates that the net flow is away from the cell.

**GHB**-is the net general-head flow volume during the time step or the stress period (L3, depend on CELLBDPRN). A positive value indicates that the net flow is into the cell and a negative value indicates that the net flow is away from the cell.

**WEL**-is the net well flow volume during the time step or the stress period (L3, depend on CELLBDPRN). A positive value indicates that the net flow is into the cell and a negative value indicates that the net flow is away from the cell.

**DRN**- is the net drain flow volume during the time step or the stress period (L3, depend on CELLBDPRN). A positive value indicates that the net flow is into the cell and a negative value indicates that the net flow is away from the cell.

**CNH**-is the net constant-head flow volume during the time step or the stress period (L3, depend on CELLBDPRN). A positive value indicates that the net flow is into the cell and a negative value indicates that the net flow is away from the cell.

**ABER**-is the budget error during the time step or the stress period (L3, depend on CELLBDPRN).

**4 CellHead.out file**

Heads are written to CellHead.out file

**IPER**- is the stress period number.

**ISTEP**- is the time step number of a stress period, this variable is valid only if CELLHHPRN=1.

**TLEN**-is the total simulation time (T).

**ILYR**-is the layer number of cells

**IROW**- is the row number of cells

**ICOL**- is the column number of cells

**XCORD**- is the X-coordinate at the center of cells (L)

**YCORD**- is the Y-coordinate at the center of cells (L)

**HEAD**-is the simulated heads of cells (L).

**5 CellDD.out file**

Drawdowns are written to CellDD.out file

**IPER**- is the stress period number.

**ISTEP**- is the time step number of a stress period, this variable is valid only if CELLDDPRN=1.

**TLEN**- is the total simulation time (T).

**ILYR**-is the layer number of cells

**IROW**- is the row number of cells

**ICOL**- is the column number of cells

**XCORD**- is the X-coordinate at the center of cells (L)

**YCORD**- is the Y-coordinate at the center of cells (L)

**DrawDown**-is the cumulative drawdown of cells (L)

**6 CellFlow.out file**

Cell-by-cell volumetric flow are saved in CellFlow.out file.

**IPER**- is the stress period number.

**ISTEP**- is the time step number of a stress period, this variable is valid only if CELLFLPRN =1.

**DLEN**- is the time span during current time step or stress period (T, depend on CELLFLPRN).

**ILYR**-is the layer number of cells

**IROW**- is the row number of cells

**ICOL**- is the column number of cells

**XCORD**- is the X-coordinate at the center of cells (L)

**YCORD**- is the Y-coordinate at the center of cells (L)

**FlowX**-is the flow volume across the right face during the time step or the stress period (L3, depend on CELLFLPRN). A positive value indicates that the flow is away from the cell and a negative value indicates that the flow is into the cell.

**FlowY**- is the flow volume across the front face during the time step or the stress period (L3, depend on CELLFLPRN). A positive value indicates that the flow is away from the cell and a negative value indicates that the flow is into the cell.

**FlowZ**- is the flow volume across the lower face during the time step or the stress period (L3, depend on CELLFLPRN). A positive value indicates that the flow is away from the cell and a negative value indicates that the flow is into the cell.