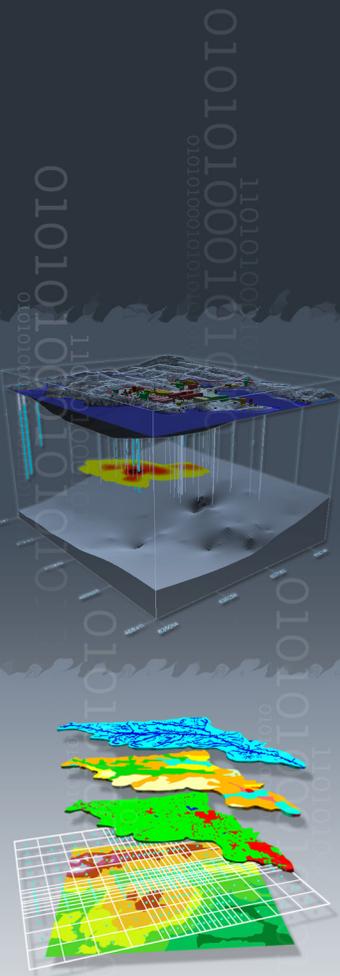




F.A.T.Q.

Frequently Asked Technical Questions
About MODFLOW-SURFACT™ and MODHMS®



Frequently Asked Technical Questions About MODFLOW-SURFACT™ and MODHMS®

Q: What are the units of length and time that MODFLOW-SURFACT™ uses?

A: *The time is user specified through the BAS file and the length is not specified so all of the parameters and data must be consistent.*

Q: Is the layer thickness sensitive to convergence? In other words, by increasing the layer thickness would you minimize convergence problems?

A: *MODFLOW-SURFACT™ is very robust and was initially designed to overcome the convergence problems associated with MODFLOW; therefore, artificially increasing the layer thickness is not necessary unless non-physical zero or negative values are used in the model.*

Q: Can I use any solver with transport in MODFLOW-SURFACT™?

A: *You must use the PCG4 solver or the PCG5 solver package with transport, though you may use any solver for the associated flow problem solution. It is, however, recommended to use the PCG4 solver or the PCG5 solver with Newton-Raphson linearization for the flow solution as well.*

Q: When would I need to use the NEWTON-RAPHSON package in MODFLOW-SURFACT™ / MODHMS©?

A: *The Newton-Raphson scheme providing quadratic convergence is used for nonlinear situations or when convergence difficulties are encountered. For unconfined or unsaturated flow problems, the use of the Newton-Raphson scheme is always recommended.*

Q: Is there a tool available to read the binary results produced by MODFLOW-SURFACT™ / MODHMS©?

A: *Yes. This tool is available directly from HGL Software Systems. Simply send your request to info@hglsoftware.com. Please specify the binary output files you need to read.*

Q: I have a 64-bit machine; can I use MODFLOW-SURFACT™ / MODHMS© on this machine?

A: *Yes. MODFLOW-SURFACT™/MODHMS© can be used on 64-bit machines. However, the source-code is compiled on a 32-bit machine.*

Q: Is it necessary to use the PCG5 solver?

A: *No. But we suggest using the PCG5 solver, because it is a robust solver and much faster than other solvers. Some users have reported the PCG5 solver to be 10 times faster than other solvers.*

Q: When do you use the OC vs. the ATO input files?

A: *The ATO package completely includes the functionality of the OC package. It is designed to maximize the time-step size for a simulation based on the ease or difficulty of convergence. User-prescribed convergence parameters limit the step sizes, number of iterations, and multiplying and dividing factors allowing the simulation a chance to move through convergence difficulties by using smaller step sizes. The step sizes are increased to adjust the prescribed value when there are no convergence difficulties. Additionally, the ATO package adjusts the step size to reach a user-defined print time value. Thus use of the ATO package is always more effective than the OC package. The ATO package is mutually exclusive from the OC package, and will override the OC package if both are on. If you have chosen both in the *.BAS file, a message will be written to the *.OUT file that the OC package isn't being used.*

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Q: The suggested defaults for viscosity and gravity have the time unit in seconds. If my model is using time in days, do I have to convert the units for viscosity and gravity, or is this already assumed in the model?

A: *The model only assumes a consistent set of units. Thus, you will need to convert all parameters to a consistent set of units before using them as input to the model.*

Q: Can MODFLOW-SURFACT™ / MODHMS© simulate flow and transport in the unsaturated zone?

A: *MODFLOW-SURFACT™/MODHMS© is capable of simulating flow and transport in the unsaturated zone using pseudo-soil or real soil relationships. It is capable of modeling flow and transport for the following:*

- 1) Advective and dispersive transport of chemical species
- 2) Linear and nonlinear retardation for each species
- 3) First-order decay and biochemical degradation of contaminants in water and soil
- 4) Generation of transformation products
- 5) Mass partitioning of a single or multicomponent contaminant with diffusive mass movement in the inactive phase
- 6) Mass partitioning of a single or multicomponent contaminant from a depleting, immobile NAPL phase with advective and dispersive transport in the active phase and diffusive transport in the inactive phase.

Q: Does MODFLOW-SURFACT™ / MODHMS© incorporate interaction between the unsaturated zone and rivers and lakes?

A: *Yes. MODFLOW-SURFACT™/MODHMS© does incorporate interaction between the unsaturated zone and rivers and lakes; however, for a rigorous treatment of surface water-groundwater interactions the integrated surface water-groundwater code MODHMS© is recommended.*

Q: What is the difference between the RECHARGE-SEEPAGE FACE BOUNDARY CONDITION package vs. the RECHARGE package?

A: *The RECHARGE-SEEPAGE FACE BOUNDARY CONDITION package allows supplied recharge into the groundwater system if the water table is below a user specified ponding elevation. This elevation corresponds to ground elevation when there is no ponding. If the water table reaches ponding elevation, the simulation allows only as much recharge to occur as is required to maintain the prescribed ponding elevations. The rest of the recharge is shed off as surface runoff. Thus recharge to the system is reduced from prescribed levels to meet maximum ponding elevation constraints. When recharge is reduced to below zero, it indicates that water is discharging the model system under seepage conditions. When the ponding elevation is above land surface, the storage term is augmented by the additional volume of ponded water.*

Additionally, the RECHARGE-SEEPAGE FACE BOUNDARY CONDITION package can be used to simulate a seepage face boundary condition by prescribing the elevation of a seepage face boundary node. If the water table is below this elevation, zero flux occurs at the boundary. If the water table reaches this elevation, the aquifer drains to maintain the seepage face elevation.

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Q: How are the pseudo-soil relations defined? Is it just a specific set of parameters for the Brook and Corey / van Genuchten soil function?

A: *Pseudo-soil functions are for Gravity-Segregated-Vertical-Equilibrium (GSVE) conditions from Huyakorn, Wu and Park, an improved sharp-interface model for assessing NAPL contamination and remediation of groundwater systems, Journal of Contaminant Hydrology, 16, 1994, 203 - 234. In SURFACT/MODHMS, they are for 2-phase air-water only, with zero residual saturation to mimic MODFLOW's GSVE simulation. Essentially, the curve has $S=1$ below the water table, and $S=0$ above it. This curve is integrated over each grid-block height to locate the unconfined water table within any grid-block. And then, $K_r = S$ gives transmissivity equal to saturated conductivity times saturated thickness of a grid-block, to exactly emulate MODFLOW conditions without inactivating dry cells, etc., and associated problems.*

Q: Is the pseudo-soil function a step function? If $S=0$ above the water table, $K_r=0$ as well, so you couldn't solve the variably saturated flow formulation? What happens with a cell which lies above the water table? $K_r \rightarrow 0$ (e.g. a constant value $1e-10$?)

A: *Pseudo-soil function is an integration of the step function, over the grid-block height. Thus, when water table is half-way up the grid-block the saturation is 0.5, when pressure-head lies at bottom of grid-block (or below it) $S = 0$, and when pressure-head lies at or above grid-block, $S = 1$. One more thing about VE as implemented in SURFACT/MODHMS - K_r is applied to horizontal flow only (to mimic transmissivity). Saturated K is used to transfer water vertically. Thus, for fully dry grid-blocks, water travels vertically under saturated K conditions. VE assumes instant, and in reality it will be less than saturated K conditions, but in that case you need to know the unsaturated zone properties, etc., and solve an unsaturated zone problem if you are interested in travel times and moisture movement thru the unsaturated zone. When a grid-block is above the water table, $K_r = 0$. Use of a small number can create unphysical flow.*

Q: When using the Van Genuchten parameters and pseudo-soil relations is the leakance recalculated?

A: *The equations for unsaturated flow are solved by MODFLOW-SURFACT™ / MODHMS®, which calculates conductance in all directions including the vertical as per a saturated conductance times a relative permeability. For pseudo-soil relations see the answer to the question above.*

Q: When using pseudo-soil or the other unsaturated flow options, the relative permeability is a function of the water saturation so does it matter if I use the real top elevation or a constant top elevation?

A: *Yes, the elevation does make a difference. The cell thickness will vary based on the elevation given, so the water saturation and the relative permeability for the pseudo-soil and the van Genuchten methods will be affected.*

Frequently Asked Technical Questions About MODFLOW-SURFACT™ and MODHMS®

Q: What head value does MODFLOW-SURFACT™/MODHMS® write for a grid cell above the water table? As I understand, there are no dry cells in MODFLOW-SURFACT™/MODHMS®, so what does it do with grid cells above the water table?

A: MODFLOW-SURFACT™/MODHMS® DOES have dry cells, only those cells are not inactive. In dry cells, it writes the heads calculated for the dry cell, which will be equal to the water-table head with no recharge. With recharge, it will be slightly higher than that, to allow for the recharge to go down to the water table. So, in essence, it is a pseudo-head, but it may be used to see where the first water-table lies since it shouldn't be much different unless confinement at the surface is large.

“Slightly” refers to the amount that satisfies the following: $q = K_v(h_2 - h_1)$ down to the water table, where q is the recharge rate and K_v is vertical saturated LEAKANCE (note for dry cells, horizontal K is zero, so there is no horizontal flow at all). So, if recharge is zero, then the h is the same from the water table up. When ball parking things during a project, I just look at the top layer heads to see where water table would lie. For rigorously calculating things, see answer to question below.

The water table can be found from the saturations in the DDN file. If saturation is zero, cell is fully dry. If saturation is one, cell is fully wet. If saturation is something in between, water-table for that cell lies in between. The saturation value represents the fraction of the cell thickness that is wet. Alternatively, if you don't have the DDN file, the heads from the HDS file can be manipulated. If the head is above the top, then the node is fully saturated. If the head is below the bottom, then the node is fully dry. If the head is between the top and the bottom, then the water table is at that level in the cell. Possibility exists for multiple water tables — one in each layer, or you can even have several dry layers between water tables.

Q: In the MODFLOW-SURFACT documentation, it mentions that if IREALSL>0 then the drawdown is replaced by saturation values. Is this still written to the .DDN file in the same format as the .DDN data?

A: Yes, saturations are written to the DDN file if IREALSL>0, in the same formats so they can be conveniently accessed by any MODFLOW postprocessor.

Q: If I am NOT simulating soil vapor flow or air-sparging, do the following parameters in the BCF4 package matter: RHOWP, RHOAP, VISW, VISG, COMPWAT, COMPARE, ATMGP, GRAV?

A: These parameters are not used or entered for water flow. For transport, if you are simulating NAPL, you will need these for the flash calculations involved therein.

Q: If the user chooses IREALS=3 or 4, then MODFLOW-SURFACT will simulate soil vapor flow above the water table elevation. What values and units does it use for the soil vapor permeability?

A: IREALS=3 or 4 simulates air flow above *and below* the water table elevation - in a sparging process, you may be injecting air below the water table level. The soil vapor permeability is calculated from the hydraulic conductivity (L/T in a consistent set of units) using viscosities (see equation 15 of chapter 2, volume 1 of the MODFLOW-SURFACT™/MODHMS® document). So the user still enters the hydraulic conductivity of the soil (as in MODFLOW), but has additional entries for the viscosities, densities, compressibilities, atmospheric pressure, etc., which are needed by equation 15 when the air phase flow problem is expressed within the MODFLOW framework.

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Q: For an air-sparging simulation, where is the air injection well information input?

A: *When simulating flow of air, you can provide a constant head (for air) boundary, or a general head boundary for air (with the head representing the equivalent freshwater head in the air phase), or a flux via the WEL or the FRACTURE WELL (FWL) file. The flux represents volume of air injected/extracted from the well node. For extraction wells, saturation of air may go to zero at /around the well due to suction. The FWL package further applies a supply/demand condition to the well for this case. FWL package over multiple nodes becomes very sensitive and has difficulties converging, as does the supply/demand condition of the FWL package (even if the well is assigned only to one layer). This is because of the high non-linearity with possible rapid change of well condition from having air, to having no air. Therefore, one layer is recommended to represent a well when using the FWL package. Further, when difficulties occur due to the supply/demand condition at the well (air extraction well node completely saturated with water), you may note the time at which it occurs and then reduce pumping manually in a simulation (as you would with a MODFLOW water flow simulation when things are going dry and not converging). Here at least, you needn't reduce it to BELOW the value at which air saturation becomes zero, but to some value close. If pumping demand is not TOO large in comparison to supply.*

Q: Is it true that you cannot find out the quantities or velocities of the vapor flow when you are simulating SVE?

A: *No, this is not true. This information is available in the CBB file. What you cannot see is the contaminant mass flux on a cell-by-cell basis for the associated transport simulation (you can see this at the boundaries); however, the storage is available on the cell-by-cell basis for each contaminant component.*

Q: What would happen in a soil vapor simulation if the water table was above the top layer elevation for some cells or below the bottom layer elevation for some cells?

A: *If the water table was above the top layer elevation, that cell has a water pressure greater than zero. If air is injected into the cell, it can enter the cell only when the air pressure is larger than the water pressure, and then, the air saturations will increase according to the moisture relations. If the water table was below the bottom layer elevation for some cells, those cells will have a residual value of water saturation, and would conduct air very well.*

Q: Does MODFLOW-SURFACT interpret the head assigned with constant heads as being the pressure head boundary condition for a vapor flow simulation? If yes, then how does it treat river boundaries and general head boundaries?

A: *This is a very interesting point regarding river boundary conditions, etc. The heads for a vapor phase simulation are the equivalent freshwater heads for the air — be it on a boundary or internal to the system. For air phase simulations; therefore, the river package, etc., should not be used (or used with caution and full understanding if you want to conceptualize something that way). You can then think of such boundaries as applying a general head condition (head dependent flux condition, with limitations on inflow or outflow) which moves air into or out of the system under that prescribed "air-head".*

Frequently Asked Technical Questions About MODFLOW-SURFACT™ and MODHMS®

Q: There was a power outage while my simulation was running. How can I restart my simulation from where it stopped?

A: MODFLOW-SURFACT™ / MODHMS© offers the capability to restart a simulation that has stopped before the completion of total simulation time (for any reason: power outage, simulation failed). For a flow and transport simulation with the FWL5 package turned on, the following changes need to be made. Depending on your simulation, you can disregard the changes that you do not need. For instance, a flow simulation with FWL5 package should disregard all transport related instructions given below, or a flow simulation without FWL5 package should disregard all transport and FWL5 instructions.

Let us say, your simulation stopped in the 10th stress period on time step 7. If you write out results to the binary files at the end of every stress period, then you can restart this simulation from the end of 9th stress period. If you write out results at the end of every time step, then you can restart this simulation from the end of 6th time step in the 10th stress period. If you write out results after every 10th time step, then you can restart this simulation from the end of 9th stress period (since 10 time steps have not been completed in stress period 10). In essence, you can restart from the most recent time step that was written out to the binary files.

Restart option needs 3 files to be created:

- 1) rootname.HDS (aquifer heads)
- 2) rootname.FH5 (FWL5 heads and concentrations)
- 3) rootname.CON (aquifer concentrations)

The above-mentioned binary files are created by MODFLOW-SURFACT™ / MODHMS©. They contain the results for the stress periods that have been completed. Copy these files onto the same folder and rename them to rootname.HDC, rootname.FHC, and rootname.COC respectively. Please note that for the restart option to work for a transport run, it is expected that FWL5 heads and concentrations are written to the FH5 file. For a flow run, FWL5 heads can be written to the HDS file itself.

Restart option need 2 files to be modified:

- 1) rootname.ATO
- 2) rootname.WL5

ATO file

The following changes need to be made to the ATO file.

- 1) TCNTNU (7th item on line 1 of ATO)
- 2) DTCNTNU (8th item on line 1)
- 3) ICNTNU (9th item on line 1)
- 4) ICNTNUC (10th item on line 1) – only for transport

TCNTNU – This is the time from where you want to restart the simulation. Please note that this is the total time of the simulation. For instance, in the example given above, assume the last time step written out was the end of the 9th stress period (monthly stress periods). The total time till end of stress period 9 is 273.0 days in the simulation. Enter 273.0 in the format F10.3.

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If you have difficulty in finding the total time for last time-step, open the OUT file in a text editor and search for the string "HEAD WILL BE SAVED ON UNIT". The last occurrence of this string will denote the last time-step at which results were written out. On finding the last occurrence, scroll down in the text editor till you find the Time Summary. The time summary is provided below the mass budgets. You will notice that the time summary has three rows of data. Row 1 corresponds to Time Step length, row 2 to Stress period time and row 3 to Total time. Note down the total time from the corresponding time unit for your model (seconds, minutes, hours, days, and years). This is the time that you should enter in TCNTNU. Please note that if you enter TCNTNU = 0, the simulation will NOT be a restart one.

DTCNTNU – This is the time-step size that is to be used for the first time step after restarting. Please note that this number will override the DELT value that you enter in data item 3 of ATO file. Also note that DTCNTNU should be in the correct time units.

ICNTNU – This is the flag and unit number for reading restart heads from an external file. The HDC file will be read on this unit number. The file will be wound to the appropriate time value (TCNTNU) to obtain the required starting heads.

ICNTNUC – This is the flag and unit number for reading restart concentrations from an external file. The COC file will be read on this unit number. The file will be wound to the appropriate time value (TCNTNU) to obtain the required starting concentrations

WL5 file

The following changes need to be made to the WL5 file.

- 1) ICNTF (7th item on line 1 of WL5 file)

ICNTF – This is the flag and unit number for reading restart heads from an external file. The FHC file will be read on this unit number. The file will be wound to the appropriate time value (TCNTNU) to obtain the required starting heads and concentrations for the FWL5 nodes. For a flow simulation, if ICNTF = ICNTNU, FWL5 restart heads are read from the HDC file. For a transport simulation, FWL5 heads and concentrations have to be read from (and written to) the FH5 file. So, ICNTF should not be the same as ICNTNU for a transport simulation.

Please note that if the restart simulation is located in the same folder as the original simulation, other output files such as OUT, CBB, DDN etc. will get overwritten with the results from the restart simulation. Also note that the output files for the restart simulation will only contain results from the restarted time onwards. It is advisable, therefore, to create a new folder to run the restart simulation OR create a backup of the older output files, in order to have all the results from the simulation.

Frequently Asked Technical Questions About MODFLOW-SURFACT™ and MODHMS®

Q: How do I use MODPATH with SURFACT / MODHMS?

A: First, you need to run your model by adding a flag in the BAS file (Basic file used by MODFLOW-SURFACT). An MPH file is produced when the flag MPHFLG is turned on in the BAS file. This flag is located on the eighth position (between columns 71 and 80) in the BAS file. Therefore, please open the BAS file in a text editor and put 1 on the 80th column to turn MPHFLG flag on. When you make a simulation run using this BAS file, an MPH file would be produced. In GW Vistas, this can be done by clicking the “create MPH file” check box.

Please make sure that you are writing every time step to the CBB file. This is done by making appropriate changes in ATO package, by writing every time step.

Before you use MODPATH you will need to edit the *.dat file in a text editor. A sample file (gvmodmp.dat) can be downloaded by clicking [here](#). The downloaded zip file contains the above mentioned dat file.

- 1) On the 2nd line of *.dat file , type the keywords “ATO” if your are using the ATO package and “FWL” only if you are using the FWL package. If you are not using FWL package, please do not type FWL.
- 2) On the 3rd line of *.dat file, type the MPH file name that was produced after the simulation run. MPH file is only produced when the MPHFLG flag is turned on in the BAS file as explained above.
- 3) Check that the maximum number of stress periods and time steps in the last line are correct if it is a transient run.

If needed please refer to <http://water.usgs.gov/nrp/gwsoftware/modpath41/ofr94464.pdf> for details on gvmodmp.dat file.

Please contact info@hglsoftware.com for the latest MODPATH version that works with SURFACT / MODHMS.

Q: I have created a steady state simulation. I want to use the steady state heads as initial conditions for my transient simulation. How do I do that?

A: Yes. MODFLOW-SURFACT™ / MODHMS© allows the use of initial heads in the form of a 2dr file. The 2dr file has the same format as the HDS file. For MODHMS users, please note that you can write out initial heads for groundwater, OLF and CHF in one 2dr file. The 2dr file, like the HDS file, has the heads in the order mentioned above, i.e. groundwater, OLF and CHF. In order to use the 2dr file, the following changes need to be made to the BAS, OLF, and CHF file. SURFACT users may please ignore the OLF and CHF packages, as they do not exist in SURFACT.

BAS file

The following change needs to be made to the BAS file.

- 1) SHEAD (data item 8 of the BAS file)

The SHEAD array is entered for each groundwater layer of the model, used as initial heads to start the simulation. Usually, the SHEAD array for one layer will consist of one line of header and multiple lines of data. In order to use initial heads from the 2dr file, only the header needs to be entered, with a negative unit number. The negative before the unit indicates that the heads are to be read from a binary file. The multiple lines of data are not necessary. Please note this should be done for each layer of the model.

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OLF file

The following change needs to be made to the OLF file.

- 1) INITIAL HEAD (data item 3 of the OLF file)

The INITIAL HEAD array is similar to the SHEAD array in the BAS file, except that there can be multiple layers for groundwater, whereas there is only one OLF layer. As was done in the BAS file, enter a negative unit number. The multiple lines of data are not necessary.

CHF file

The following change needs to be made to the CHF file.

- 1) INITIAL HEAD (data item 18 of the CHF file)

The INITIAL HEAD array is similar to the SHEAD array in the BAS file, except that there can be multiple layers for groundwater, whereas there is only one CHF layer. As was done in the BAS file, enter a negative unit number. The multiple lines of data are not necessary.

FWL5 initial heads can be prescribed in a similar way by using a 2df file. The 2df file is similar in format to the FH5 (FWL5 heads) file.

In order to read initial heads from a 2df file, the following changes need to be made to the WL5 file.

- 1) INITH5 (6th item on line 1 of WL5 file)

INITH5 should be greater than 0, and it is the unit number on which the 2df file will be read. Please note that FWL5 heads can also be read from a 2dr file, in which case INITH5 should be made the same as the unit number entered in the BAS for SHEAD.