Benefits of Using MODFLOW-SURFACT in Visual MODFLOW

MODFLOW-SURFACT has effectively addressed the primary shortcomings and limitations of the USGS public domain versions of MODFLOW by extending the physical modeling capabilities of the standard USGS MODFLOW code for subsurface flow calculations and enhancing the robustness and efficiency using superior numerical schemes.

The **Basic Flow** version includes:

- New Block-Centered Flow (BCF4) Package handles complete drying and re-wetting of grid cells using pseudo-soil water retention functions to account for vertical flow components throughout the domain and delayed yield response.
- Recharge Seepage Face (RSF4) Package provides the capability to prevent water table build-up above ground surface
- Fracture-Well (FWL4) Package ensures well pumping rates are not compromised by water table fluctuations during over-pumping conditions
- Adaptive Time-Stepping and Output Control (ATO4) Package automatically optimizes the time-step size during transient simulations, making the step size incrementally smaller during rapidly changing conditions, or incrementally larger during more stable conditions.
- New Preconditioned Conjugate Gradient Solver (PCG4) Package includes a faster preconditioning method.
- Newton-Raphson Linearization and Backtracking (NRB1) Package stabilizes the solution for highly non-linear conditions.

The Advanced Flow version includes all of the above capabilities, plus the option to use a more rigorous formulation for simulating 3D variably saturated flow. This option can be used to simulate variably saturated groundwater flow, or variably saturated soil vapor flow.

The following sections provide a more detailed description of these key features and provides some examples to clearly demonstrate the benefits of using MODFLOW-SURFACT. The majority of the technical details are excerpts from the MODFLOW-SURFACT User's Manual and additional details can be provided upon request.

The New Block-Centered Flow (BCF4) Package

<u>Background:</u>
In the early versions of MODFLOW-88, when a cell became dry (i.e. when the water table dropped below the bottom elevation of the grid cell) it was shut-off and omitted from the remainder of the simulation. In 1991 the USGS introduced a new Block-Centered Flow Package (BCF2) with a cell rewetting option that allowed for resaturation of the dry cells. The BCF2 rewetting scheme utilizes the head values in the neighboring grid cells to determine whether a dry cell should be re-wetted. Unfortunately, the BCF2 rewetting option is prone to convergence and stability problems during rewetting or when withdrawals dry up the respective cells (McDonald et al., 1991).

<u>Benefits of the BCF4 Package:</u>
The BCF4 Package in MODFLOW-SURFACT handles complete drying and re-wetting of grid cells using a pseudo-soil water retention functions (Pseudo-soil functions) to account for vertical flow components throughout the domain and delayed yield response. Instead of shutting off cells when the water table drops below the cell bottom, the Pseudo-soil functions are automatically generated to reduce the unsaturated flow problem to one of seeking the water table level. The formulation has been designed to provide accurate delineation of the water table and capture the delayed yield response of an unconfined system to pumping and recharge.

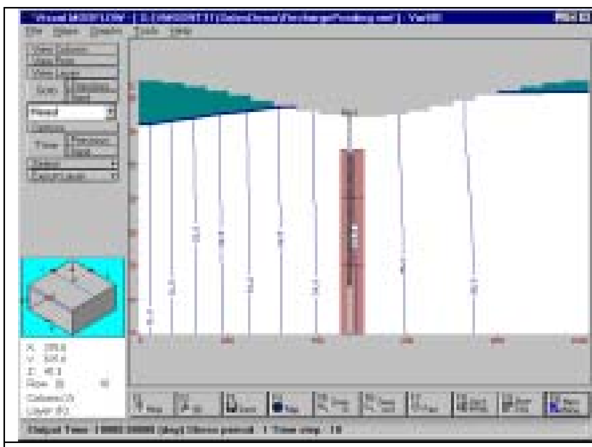
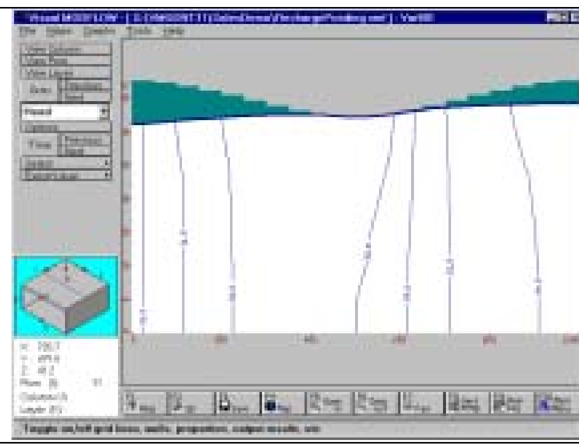
MODFLOW-SURFACT does have dry cells, only those cells are not inactive. In dry cells, it writes the heads calculated for the dry cell", which will be equal to the water-table head with no recharge. With recharge, it will be slightly higher than that to allow for the recharge to go down to the water table.

The Recharge Seepage-Face (RSF4) Package

<u>Background:</u>
The Recharge Package (RCH1) used in the standard USGS versions of MODFLOW simply allows you to specify a recharge value and the layer in which this recharge value is being applied. Unfortunately, the RCH1 package has certain limitations when dealing with unconfined systems. In the real-world, if an unconfined aquifer saturates to the ground surface, the capacity of the aquifer to absorb the specified recharge is reduced, with the remaining recharge being shed as surface runoff. Unfortunately, the RCH1 package is incapable of handling such a situation, and instead the water table simply continues to build up above the ground surface as the same amount of recharge is continually applied to the system. If the solution converges, it usually results in a water table elevation high above the ground surface. Anyone living inside the model domain would have to be good swimmers!

<u>Benefits of the RSF4 Package:</u>
The primary advantage of the RSF4 Package is the ability to specify a ponding elevation representing the upper boundary of the water table. The ponding elevation effectively represents the maximum water table elevation, whereby the recharge entering the system is automatically reduced in order to prevent the water table rising above the specified ponding elevation.

This benefit is effectively demonstrated in the following comparison where the same model was run first using MODFLOW-2000, and then run again using MODFLOW-SURFACT with the RSF4 Package and a ponding elevation set to 0.0 m above ground surface.

	
(A) Model run using MODFLOW-2000 with the RCH1 Package	(B) Model run using MODFLOW-SURFACT with the RSF4 Package

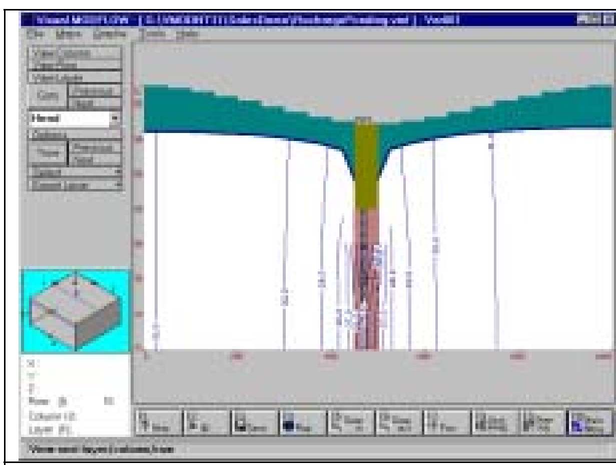
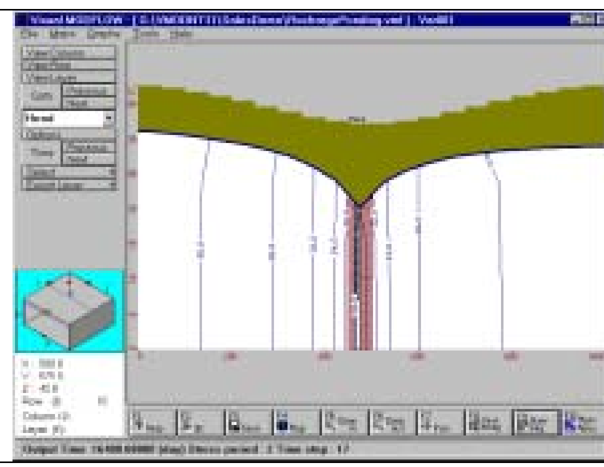
In the MODFLOW-2000 modeling results shown in Figure A, the water table rises 4 – 5 m above the ground surface in the area where the ground surface is depressed, while in the MODFLOW-SURFACT model the water table meets but does not exceed the ground surface. Clearly, MODFLOW-SURFACT is able to produce a more physically realistic representation of the real-world conditions.

The Fracture-Well (FWL4) Package

Background:
The standard USGS versions of MODFLOW allow you to assign an extraction (or injection) rate to individual grid cells in the model. For the sake of this document, the grid cells assigned as well boundary conditions will be referred to as ‘well cells’. If a pumping well is screen across several model layers, it is up to the user to determine how the extraction rate is proportioned among the well cells from each layer. Furthermore, if the pumping well is over-pumping from the aquifer and the water table drops below the bottom of the uppermost well cell, the ‘dry’ well cell is deactivated and the pumping rate from this cell is omitted from the calculation. If the water table rises above the bottom of the well cell in the next iteration, the well cell is reactivated and the extraction rate from this cell is re-introduced to the model. As you can imagine, this often results in oscillatory solutions where the well cell cycles between dry and wet as the extraction rate from this cell is repeatedly turned on and off. In addition, if the model does converge to a solution, there are no warnings from MODFLOW to indicate the total well pumping rate has been reduced, so the results may be misleading (i.e. you may think the results indicate the response of a well pumping at a rate of 500 cubic meters per day, but one of the well cells is dry and the actual pumping rate is only 333 cubic meters per day).

Benefits of the FWL4 Package:
The FWL4 Package allows you to truly simulate a pumping well that is screened across multiple model layers. The FWL4 package connects the grid cells intersecting the well screen by representing the pumping well as a one dimensional finite diameter fracture tube spanning the length of the well screen. You specify an extraction rate for the pumping well and the water is effectively removed from the bottom of the well screen. The volumetric fluxes from each individual cell associated with the well are automatically calculated according to the length of the well screen in the cell and the transmissivity of the cell at each time step. This approach ensures the total extraction rate from the pumping well is ALWAYS honored unless the water table drops below the bottom of the well screen (i.e. the entire well goes dry).

This benefit is effectively demonstrated in the following comparison where the same model was run first using MODFLOW-2000, and then run again using MODFLOW-SURFACT with the FWL4 Package and a well radius of 0.02 m.

	
(A) Model run using MODFLOW-2000 with the standard WEL Package	(B) Model run using MODFLOW-SURFACT with the FWL4 Package

In the MODFLOW-2000 modeling results shown in Figure A, the pumping well over-pumps the unconfined aquifer causing the water table to drop below the bottom elevation of the uppermost well cell. This deactivates the uppermost well cell and reduces the total extraction rate of the pumping well from 500 m^3/day down to 333 m^3/day. However, in the MODFLOW-

SURFACT model the water table also drops below the bottom elevation of the uppermost well cell, but the extraction rate of the pumping well is maintained at 500 m^3/day and produces a more realistic and accurate representation of the drawdown caused by the pumping well.

The Adaptive Time-Stepping and Output Control (ATO4) Package

Background:
In the standard USGS versions of MODFLOW, the time domain for transient simulations is discretized using a backward-difference formulation, with time-step sizes for each stress period being predetermined by the user prior to running the model. Typically, the time steps are incremented exponentially with the highest density of time-steps occurring near the beginning of the stress period where the most rapid changes to the system are occurring. However, if the solver fails to converge in a given time step, the solution simply aborted with no additional efforts to address the problem. In addition, the predetermined time steps may be inefficient to solve the problem, even when convergence is achieved.

Benefits of the ADO4 Package:
The ADO4 Package automatically selects the time-step size depending on the anticipated non-linearities of the system during a given calculation. If the anticipated non-linearities are not significant, a larger time step is selected to aggressively move forward with the solution. If anticipated non-linearities are severe, a smaller time step size is selected to ensure convergence for a time step. In the event a solution fails to converge for a given time step, the time step size is further reduced and the solution is repeated. The factors by which the time step sizes are increased and descreased are controlled by the user. The minimum time step size is also controlled by the user to prevent an endless loop of decreasing time steps.

The end result is a solution that is usually faster and more accurate than with the standard USGS versions of MODFLOW.

The New Preconditioned Conjugate Gradient (PCG4) Solver Package

Background:
The PCG2 solver used in the standard USGS versions of MODFLOW uses either a least squares polynomial preconditioner presented by Saad (1985) or the optimal Chebyshev polynomial preconditioner of Meyer et al. (1989). These schemes were chosen primarily on computer storage and memory considerations and often perform poorly on large scale field studies.

Benefits of the PCG4 Solver Package:
The PCG4 Package uses partial LU decomposition as a preconditioner. This method is simple and very robust, but it does require more computer storage and memory than the PCG2 Package. However, in today's day and age, computer memory and CPU speed should no longer be considered as limiting factors.

The Newton-Raphson Linearization with Backtracking (NRB1) Package

Background:
The standard USGS versions of MODFLOW utilize a Picard iteration scheme for solving the flow equations. However, this scheme is inadequate to handle highly the nonlinear conditions often encountered with unconfined aquifers and often results in excessive iterations or failure of the solution.

Benefits of the NRB1 Package:
The NRB1 package integrates the Newton-Raphson iteration scheme with a backtracking algorithm to stabilize the Newton iterations by controlling the step-size. The backtracking scheme limits the increase in residuals at any iteration while an under-relaxation technique assists with oscillatory behavior of the solution between iterations.