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Modeling Surface Water-Groundwater Interaction with MODFLOW: Some Considerations

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Abstract

The accuracy with which MODFLOW simulates surface water-groundwater interaction is examined for connected and disconnected losing streams. We compare the effect of different vertical and horizontal discretization within MODFLOW and also compare MODFLOW simulations with those produced by HydroGeoSphere. HydroGeoSphere is able to simulate both saturated and unsaturated flow, as well as surface water, groundwater and the full coupling between them in a physical way, and so is used as a reference code to quantify the influence of some of the simplifying assumptions of MODFLOW. In particular, we show that (1) the inability to simulate negative pressures beneath disconnected streams in MODFLOW results in an underestimation of the infiltration flux; (2) a river in MODFLOW is either fully connected or fully disconnected, while in reality transitional stages between the two flow regimes exist; (3) limitations in the horizontal discretization of the river can cause a mismatch between river width and cell width, resulting in an error in the water table position under the river; and (4) because coarse vertical discretization of the aquifer is often used to avoid the drying out of cells, this may result in an error in simulating the height of the groundwater mound. Conditions under which these errors are significant are investigated.

Introduction

According to Furman (2008) and Barlow and Harbaugh (2006), the most commonly used numerical model to simulate surface water–groundwater interactions is MODFLOW. However, there are also a number of more sophisticated models that include a more realistic physical coupling between surface water and groundwater. This study focuses on the influence of conceptual assumptions on the simulation of the interaction between losing streams and groundwater using MODFLOW. Such conceptual assumptions are embedded in the way rivers are assigned to the model grid or in the equations used to calculate infiltration fluxes. We discuss and quantify the influence of such assumptions and point out in what situations they will affect the modeling outcome. Most of the issues we talk about are also relevant for gaining streams. However, the simulation of gaining streams adds additional complexities (e.g., the influence of neglecting seepage of groundwater along a riverbank of a gaining stream) and their discussion is not within the scope of this paper.

Modeling Streamflow in MODFLOW

Numerous streamflow packages with different levels of complexity have been developed for MODFLOW. We limit our discussion to streamflow packages developed by the USGS because of their availability and their widespread acceptance. The first streamflow package was

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the River Package RIV (McDonald and Harbaugh 1988). In the River Package, rivers are conceptualized as head-dependent flux boundaries. Follow-up packages to the River Package are the Stream Package STR1 (Prudic 1989), the Streamflow Routing Package SFR1 (Prudic et al. 2004), and the Streamflow Routing 2 Package SFR2 (Niswonger and Prudic 2006). Several conceptual assumptions of the River Package are the same in all streamflow packages.

In all of MODFLOW's streamflow packages, the flow from a river to the aquifer is calculated differently for hydraulically connected and disconnected systems. In MODFLOW terminology, the groundwater is *hydraulically connected* if the water table is above the elevation of the base of the streambed sediments. In this case, the exchange volumetric flux Q_{MF} [L^3T^{-1}] between the river and the groundwater is calculated using

$$Q_{MF} = \frac{K_c L w}{h_c}(h_{riv} - h) = c_{riv}(h_{riv} - h) \qquad (1)$$

where K_c [LT^{-1}] is the hydraulic conductivity of the clogging layer, L is the length of the river within a cell [L], w is the width of the river [L], h_c [L] is the thickness of the clogging layer, h_{riv} is the hydraulic head of the river [L], h is the groundwater head, and c_{riv} [L^2T^{-1}] is the conductance of the clogging layer (McDonald and Harbaugh, 1988). The hydraulic conductance is a lumped parameter summarizing the geometry of the river and the clogging layer as well as its hydraulic conductivity.

If the water table h is below the elevation of the streambed bottom z_a ($h < z_a$), the surface water-groundwater system is considered *hydraulically disconnected* in MODFLOW. In this case, the volumetric infiltration flux Q_{MF} from the river to the aquifer is calculated using

$$Q_{MF} = c_{riv}(h_{riv} - z_a) \qquad (2)$$

We analyze four important aspects of model conceptualization in MODFLOW.

- The unsaturated zone is not considered. Equation 2 assumes that the pressure at the bottom of the clogging layer is zero and therefore the hydraulic head at this point is equal to the elevation head.
- A river reach can only be assigned to one specific grid cell and therefore cannot be discretized horizontally, resulting in a uniform exchange flux under the river.
- Because a river can only be tied to one grid cell, there is often a mismatch between river width and the underlying grid cell. In a regional model, for example, the grid cells a river is tied to are often much wider than the physical width of the river.
- In order to avoid dry model cells, a coarse vertical discretization of the aquifer is often used. It is therefore assumed that within a grid cell the hydraulic head does not vary vertically. However, under an infiltrating river this might not be the case.

These assumptions and conceptual constraints can lead to errors in the groundwater mound and to errors in the infiltration fluxes:

- No negative pressure gradients are considered (point 1, above) and therefore gravity drainage through the streambed is assumed. However, in disconnected systems, suction occurs at the bottom of the streambed. Therefore, MODFLOW underestimates infiltration fluxes for disconnected rivers.
- As a consequence of neglecting the unsaturated zone and assigning a river to one grid cell only (point 2), a river in MODFLOW is either connected or disconnected, while in reality transitional stages between the two flow regimes exist. These transitional stages cannot be modeled in MODFLOW.
- A mismatch between river width and the grid cell results in an error of the water table, because the exchange rates between surface water and groundwater are distributed over the area of the grid cell (point 3). In reality, however, the water table depends on the distribution of infiltration fluxes across the river and should not be related to the size of the grid cell.
- If the vertical flow component is significant, it must be calculated using a fine vertical grid. Using a coarse vertical discretization (point 4) results in an error in head.

Also, by neglecting the unsaturated zone, water infiltrating from the river is added to the groundwater immediately. In a disconnected system, however, the storage and flow of water within the unsaturated zone may be important and the time delay between infiltration and recharge can be significant. This time delay is not explicitly examined in this paper. However, in the SFR2 package, a time lag between infiltration from the river and groundwater recharge is introduced by approximating the flow (negative pressure gradients are not considered) through the unsaturated zone using a kinematic wave approximation of the Richards equation.

The above-mentioned conceptual assumptions are made in all streamflow packages, and are justified for a wide range of applications. However, it is important to quantify when they are or are not applicable as well as to further understand the consequences of these assumptions for quantifying surface water–groundwater interaction in losing streams. A systematic analysis of these assumptions is therefore required to ensure that an appropriate modeling code is used to simulate a specific problem.

Model Simulations

The starting point of this analysis is an example of a connected, losing river. We assume no subsurface flow parallel to the river. Therefore, the flow from or to the river is perpendicular to the river channel. If the water table is lowered, the infiltration flux from the surface water body to the aquifer increases. However, initially, the flow between the river and the aquifer remains saturated (losing connected). If the water table is dropped further, the flow between the river and the aquifer can become unsaturated. A necessary but not sufficient condition required for unsaturated flow to occur is that the hydraulic conductivity of the streambed is small compared to the hydraulic conductivity of the aquifer. (If the hydraulic conductivity of the streambed is lower than the underlying aquifer, the streambed is referred to as the clogging layer.) Brunner et al. (2009a) developed an exact criterion to determine whether the flow can become unsaturated or not. If an unsaturated zone can develop, the water table can be lowered to an extent where the infiltration rate effectively becomes independent of a further decrease in the water table. At this point, the infiltration flux of the stream is the highest possible (for a given stream stage) and the stream is said to be hydraulically disconnected from the groundwater system. Only if the water depth in the river changes or the water table rises and reconnects the system will the infiltration rate change.

In the following, we simulate the relation between different stages of the water table and the infiltration rate under a straight river (this corresponds to the example studied in Brunner et al. [2009a]) with both MODFLOW 2000 (Harbaugh et al. 2000) and HydroGeoSphere (HGS) (Therrien et al. 2006). The simulations are all steady state and therefore represent a series of different flow regimes between connected and disconnected. We carry out all of our MODFLOW calculations using the River Package because most of the assumptions we discuss for this package apply to all USGS streamflow packages. HGS simulates both saturated and unsaturated flow. The ability of HGS to simulate flow in the unsaturated zone using the Richards equation as well as the disconnection of surface water and groundwater has been tested in Brunner et al. (2009a). Moreover, Brunner et al. (2009a) compared the free water surface under an infiltrating layer calculated with HGS and an analytical solution (Schmitz and Edenhofer 2000) not based on any form of linearization. The agreement between the two approaches was excellent. HGS is therefore considered as the control experiment for comparison in this paper. Figure 1 shows the basic model setup.

In the variably saturated formulation set up in HGS, a relation between pressure and hydraulic conductivity describing the unsaturated zone has to be defined. We used the van Genuchten approach with the parameters $\alpha = 14.5\ \mathrm{m}^{-1}$ and $\beta = 2.68$. These parameters are typical values for sand (Carsel and Parrish 1988). The river in HGS is represented as a constant head boundary above the clogging layer. This is an identical approach to the River Package in MODFLOW. In order to correctly simulate the unsaturated zone, the aquifer must be finely discretized vertically in HGS. In MODFLOW, there are limits to the vertical discretization because model cells can fall dry (the issue of dry cells is discussed later). In order to quantify the impact of the coarse discretization in MODFLOW, the model set up in HGS is discretized finer both horizontally ($\Delta x = 1$ m) and vertically (with a vertical discretization of 10 cm between z = 115 m and z = 120 m and with 5 m between z = 0 m and z = 115 m).

The uniform horizontal discretization Δx of the model domain in MODFLOW is 10 m and is equal to the width of the river. Vertically, the MODFLOW model is discretized with 12 layers each of 10 m thickness. The model length in the direction of the river is 10 m (Δy), represented by a single row. The aquifer is 120 m high in the z direction and the elevation of the bottom of the clogging layer z_a is also 120 m. The hydraulic conductivity of the aquifer K_a is set to 1 m/d. Homogeneous and isotropic conditions are assumed. The height of the clogging layer h_c is 0.3 m, and its hydraulic conductivity K_c is 0.1 m/d. The depth d of the river is 0.5 m and its width w is 10 m. The river is straight, leading to a river length of 10 m. For some simulations, HGS is not used but instead different setups within MODFLOW are constructed and compared. The differences to the initial setup described above are mentioned in the corresponding paragraphs.

For both HGS and MODFLOW simulations the head at the lateral boundary is lowered and the steady-state infiltration rate is calculated. The system is initially losing connected. The head at the lateral boundary is lowered until the river is disconnected from the groundwater. The groundwater is disconnected from the surface water when the infiltration flux no longer significantly changes in response to a falling water table. In MODFLOW, this is the case as soon as the water table drops below the elevation of the riverbed bottom. In Figure 2, the effect of lowering the head at the lateral boundaries for the two models is illustrated. In HGS, the groundwater is not disconnected as the water table begins to fall below the bottom of the clogging layer. Rather, a transition between connected and disconnected is present and the system in HGS is considered disconnected when an additional increase of ΔH no longer significantly changes the infiltration rate. In the transition between connected and disconnected flow, the flow regime between the river and the groundwater is partly unsaturated while the infiltration rate remains a function of the water table (Fox and Durnford 2003). Brunner et al. (2009a) showed that

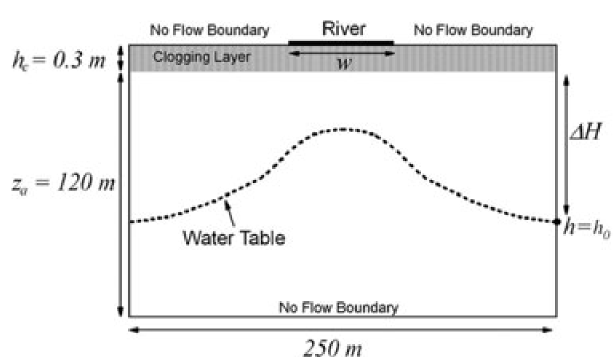

Figure 1. Model setup used in both MODFLOW and HGS. The horizontal extent of the model is 250 m. The datum $z = 0$ is defined in the lower left corner. Constant head boundaries are defined at the edges of the model domain between $z = 0$ and $z = h_0$. The midpoint of the river is defined in the center of the model domain. We assigned the entire model domain a thickness of 10 m.

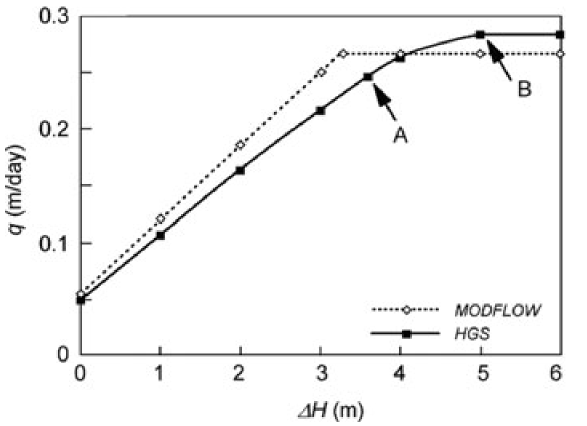

Figure 2. Steady-state infiltration rates of the river as a function of ΔH calculated in MODFLOW and HGS. ΔH is the difference between the hydraulic head at the constant head boundary and the elevation of the top of the aquifer. Point A represents the beginning of the transition zone (beginning of desaturation at the edge of the river). At point B, disconnection is reached.

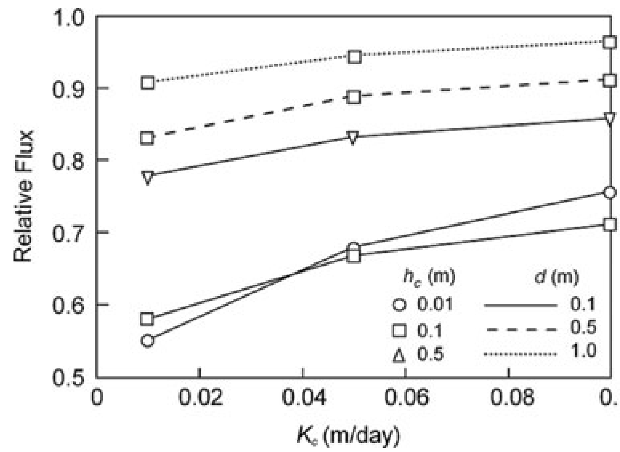

Figure 3. Illustration of the influence of neglecting the suction under the clogging layer for disconnected systems. The relative flux shown on the y-axis is the ratio of the infiltration flux of a disconnected system calculated by MODFLOW ($\gamma_p^* = 0$) to the infiltration flux calculated with a model considering the unsaturated zone. The aquifer material was assumed to be sand. For better readability, only five of the nine possible parameter combinations are shown in this graph.

this transition is related to both the buildup of a capillary zone (negative pressure gradients) above the water table as well as to the geometric properties of the river. Brunner et al. (2009b) showed that different transitional pathways exist and that they can significantly influence how changes in the water table affect the infiltration rates.

Compared to MODFLOW, the simulations carried out with HGS show a higher infiltration flux at full disconnection and the transition between connected and disconnected is smooth. Some of the above-mentioned assumptions and conceptual aspects of MODFLOW explain the two differences between MODFLOW and HGS. In the following, we discuss and quantify these assumptions in greater detail.

Underestimation of Infiltration

In MODFLOW's stream and river packages (including SFR2), the unsaturated zone is modeled without considering negative pressure gradients. However, if an unsaturated zone is present under the clogging layer, a suction γ_p [L] occurs and this suction increases the flux through the clogging layer. Using Darcy's law,

$$q = \frac{K_c}{h_c}(h_{riv} - z_a - \gamma_p) = \frac{K_c}{h_c}(h_c + d - \gamma_p) \qquad (3)$$

where $z_a - \gamma_p$ is the hydraulic head below the streambed sediments, and so the left-hand side of this equation is simply Darcy's law for flow through the streambed sediments. The difference between the hydraulic head of the river h_{riv} and the elevation of the bottom of the clogging layer z_a is equal to the sum of the river depth d and the height of the clogging layer h_c. In MODFLOW, γ_p is zero and Equation 3 reduces to Equation 2. Therefore, if the values of hydraulic conductivity of the streambed and its geometrical properties are available and used as input data, the infiltration flux will be underestimated in the River Package if an unsaturated zone is actually present. In practice, values of streambed hydraulic conductivity and its vertical extent are hard to determine and are often unknown.

It is apparent from Equation 3 that neglecting the unsaturated zone is justified only if $|\gamma_p| \ll h_c + d$. In Figure 3, the influence of neglecting the suction under the clogging layer on the infiltration rate of a disconnected system is illustrated for different combinations of d, h_c and K_c. The suction γ that occurs at disconnection is defined as γ_p^*. The parameters used in the van Genuchten equations (van Genuchten 1980) are based on Carsel and Parrish (1988) ($\alpha = 14.5$ m^{-1} and $\beta = 2.68$, K_a =7.1 m/d. A relatively large value of K_a was chosen to demonstrate this effect because it is less noticeable if K_a is close to K_c).

The magnitude of γ_p^* depends on the soil type, the saturated hydraulic conductivity of the aquifer, and the gravity flux through the clogging layer. γ_p^* is always larger than the air entry value of the aquifer material. In the parameter combinations we presented in Figure 3, the underestimation of flow is up to a factor of 1.85 (relative flux 0.54). Osman and Bruen (2002), however, discussed parameter combinations where the decrease was about a factor of three. The effect of the unsaturated zone will diminish when the river is deep or the clogging layer is thick. In the range of the simulations we carried out, the increase of flux as a result of suction was small (5% or even less) when the sum of the river depth and the height of clogging layer river was above 1 m.

Uniform Infiltration Rates under a River and Absence of Transition Zone

If a river in MODFLOW is represented with a single cell it is either completely connected or completely disconnected. In two and three dimensions, however, a

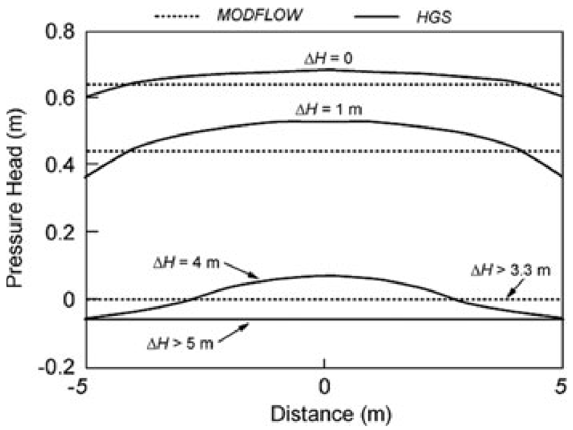

Figure 4. Pressure distribution across the river between $-w/2$ and $w/2$ (in this case river width $w = 10$ m) measured at the bottom of the clogging layer for different values of ΔH for MODFLOW and HGS. HGS gives a distribution of pressure under the riverbed, while MODFLOW presents only one data point. In the HGS simulation shown for $\Delta H =$ 4 m, different states of connection under the clogging layer can be identified. In this case, at the edge of the river, the flow is unsaturated ($\gamma_p < 0$), while the flow in the center remains saturated ($\gamma_p > 0$). The model setup and the parameters are the same as shown in Figure 1.

groundwater mound develops under the recharging surface water body, and the pressure distribution is a function of the location under the riverbed. This nonuniform pressure distribution causes different states of connection at different points in space and manifests itself as an extended transition zone. The pressure distribution under the clogging layer is uniform only when a system is disconnected. Figure 4 illustrates these differences.

In the simulations shown in Figure 4 it is apparent that the pressure head in MODFLOW is very close to the average pressure head under the clogging layer for HGS. The results of many simulations (considering a wide range of different parameter combinations, including wide rivers with a large transition zone) suggest that the average pressure in MODFLOW was close to the average value of the finely discretized HGS model. The difference of the infiltration flux for different values of ΔH could be explained as a result of neglecting γ_p in MODFLOW and is only marginally related to the assumption of uniform pressure under the clogging layer. This suggests that the assumption of uniform pressure does not significantly influence the total exchange flux, and for many regional models this assumption is therefore justified. However, the missing horizontal discretization within a river cell has an effect on the groundwater mound if the physical width of the river does not exactly match the width of the river cell, as described below. (We are aware that it is possible to represent a river as a series of parallel rivers tied to a series of grid cells, allowing for horizontal discretization in the River Package. In all other streamflow packages, however, the river depth is calculated and not prescribed and splitting a river up into several parallel rivers is not straightforward.)

As illustrated in Figure 2, the MODFLOW simulations do not feature a transition between connected and disconnected regimes. As mentioned above, there are two reasons for this difference: The first one is the absence of negative pressures in MODFLOW. As the water table drops below the clogging layer, the infiltration rates continuously approach their maximum values. This is a smooth function and cannot be reproduced in a model that does not consider capillary pressure gradients. The second reason is due to the absence of horizontal discretization of the river. Therefore, in MODFLOW a river is either fully connected or fully disconnected while in reality the state of connection can vary across a river.

Error in Water Table due to Mismatch of River Width and Grid Cell Size

There is often a mismatch between the river width w and the width of a grid cell Δx. (In fact, there is always a mismatch in a finite difference scheme if the river is not straight.) While the volumetric infiltration flux $Q[\mathrm{L}^3\mathrm{T}^{-1}]$ of a disconnected system is not affected by this mismatch, the infiltration flux $q[\mathrm{LT}^{-1}]$ is. This is an important difference because the infiltration rate and the geometry of the system are the relevant parameters for determining the groundwater mound under an infiltrating layer. If the area of the grid cell is much greater than the area of the river within it, then the infiltration flux $q[\mathrm{LT}^{-1}]$ and therefore the height of the groundwater mound beneath the river will be underestimated. Because the calculation of the infiltration flux is based on the head difference between the river and the groundwater, the calculated infiltration fluxes are systematically biased if the river and cell width do not match.

Consider two configurations of a straight river in MODFLOW. The hydraulic parameters are identical, but the horizontal size of the grid cell the river is tied to differs. We define the horizontal dimension of the river cell as a multiple α of the real river width w such that $\Delta x = \alpha w$. At disconnection, the volumetric infiltration Q is independent of α while the infiltration rate q is a function of α:

$$q = \frac{Q}{\Delta x \Delta y} = \frac{Q}{\alpha w \Delta y} \quad (4)$$

It is readily apparent from Equation 4 that different values of α influence the infiltration rate q and hence the groundwater mound. In Figure 5, the hydraulic head under an infiltrating layer of the width w is plotted as a function of x for different values of α. If the river is tied to a grid cell with a width smaller than the river ($\alpha < 1$), the height of the mound under the river is overestimated. If the width of the grid cell is larger than the width of the river ($\alpha > 1$), the mound is underestimated. In a typical regional model, α is larger than 1. The largest error in head is made directly beneath the center of the river. For illustrative purposes, some parameters in Figure 5 deviate from the ones used to generate Figures 3 and 4: $L = 500$ m, $w = 20$ m, $d = 0.4$, $h_c = 0.4$, $K_c = 0.1$ m/d, $K_a = 1$ m/d. All other parameters as well as the vertical

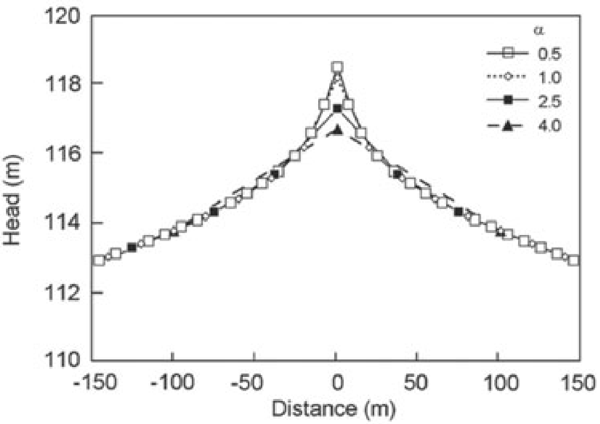

Figure 5. Groundwater mound under a river with the same hydraulic conductance but different sizes of the river cell (calculated using MODFLOW). The largest deviations are found directly under the river. The horizontal discretization along x is varied according to the value of α, where $\alpha = \Delta x/w$. In this particular setup, $\alpha = 1$ corresponds to $\Delta x = w = 20$ m.

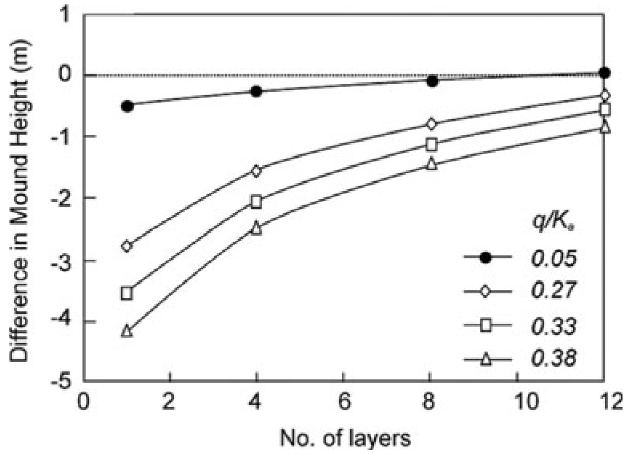

Figure 6. Influence of the vertical discretization of the model domain on groundwater mound height for different q/K_a ratios. The x-axis shows the number of layers that were used in the vertical discretization of the model domain (with a height of 120 m). The discretization is regular over the entire model domain. The difference in head is calculated by subtracting the head obtained using HGS from the values obtained in MODFLOW. h_0 is set to 111 m in MODFLOW and HGS. All the cases shown in the figure are hydraulically disconnected.

discretization are the same as in the previous mentioned example.

In disconnected systems, the water table outside of the river is not affected by this error in head as long as the influence of grid discretization does not affect the state of connection. For the examples shown in Figure 5, the error in head is not sufficient to change the state of connection and the groundwater mound is only in error directly under the river while the hydraulic heads outside of the river closely match. However, this is not the case for connected systems. This is because in connected systems the infiltration flux is dependent on the hydraulic head under the river and an error in this head results in an error of the infiltration flux and affects the groundwater mound over the entire model domain.

Error in Water Table due to a Coarse Vertical Grid

The vertical discretization of the aquifer (layer thickness in MODFLOW terminology) also influences the groundwater mound under a recharging surface area. In principle, an aquifer can be modeled as one single layer. In many cases, this is a convenient setup because no or few cells dry out as a consequence of a dropping water table during the simulation. (A grid cell falls dry if the hydraulic head falls below the bottom elevation of the grid cell.) Dry cells cause convergence problems and once a cell has fallen dry it remains dry unless it is actively reactivated, for example, by the rewetting package in MODFLOW. However, while the rewetting package allows the model to "rewet" dry cells during the simulations, this can cause convergence problems (Doherty 2001). While a very coarse vertical discretization of the grid reduces the possibility of cells drying out, no vertical variation of the hydraulic head can occur within a cell. This will cause errors in the groundwater mound if the vertical component of flow is significant. The ratio of vertical infiltration rate to the hydraulic conductivity of the aquifer gives some information on the importance of the vertical component of flow. In Figure 6, the difference between a finely discretized model in HGS and MODFLOW is shown for different ratios of q/K_a and different vertical discretizations. The parameters used to define the stream and streambed are identical to those used in Figures 2 and 3. The changes of the q/K_a ratio were created by a variation in K_a. The largest errors are found for a high q/K_a ratio where only one model layer is used.

All the above-mentioned conceptual assumptions of MODFLOW result in a model that is easy to use and that does not require large computing systems or long run times. The difference in run times between MODFLOW and HGS is significant. For example, a model run to calculate the results in Figure 4 (curve for $\Delta H = 4$ m) was 37 times faster in MODFLOW than it was in HGS. The choice of model will therefore be a tradeoff between the faster runtimes in MODFLOW and increased accuracy in models such as HGS.

Discussion and Conclusions

Some of the well-known assumptions embedded in the conceptualization of MODFLOW related to surface water-groundwater interaction have been analyzed. In particular, we showed the following: (1) Neglecting negative pressure gradients leads to an underestimation of the infiltration flux. (2) Because rivers are assigned to only one grid cell, the infiltration flux under a river is uniform while in reality this is only true for disconnected systems. (3) The size of the single grid cell a river is assigned to influences the infiltration flux, and (4) The vertical discretization of the aquifer affects the infiltration flux. A simple river-aquifer system was modeled. Groundwater flow was assumed to be perpendicular to the river, allowing for a 2-D conceptualization. The aquifer was assumed to be homogeneous and isotropic and the analyses are steady state. We are aware that this setup is simplified, but the issues that are noted in this paper do not change within a more complex system. For example, a mismatch between river width and cell width will result in differences in the infiltration rate, irrespective of whether the aquifer is homogeneous or heterogeneous or the system is transient or in steady state. Even though all our simulations are for losing streams, the considerations on vertical discretization of the aquifer and the horizontal discretization of the river are also relevant for gaining streams. However, additionally complexities arise in the simulation of gaining streams (e.g., seepage along the riverbank). Most of the conceptual considerations we have described above can go unseen through calibration. This can be problematic because the model will produce biased predictions if it is used in any situation other than those for which it was calibrated.

Acknowledgments

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