Two helpful ideas for users of MODFLOW

A. SPALVINS, J. SLANGENS, R. JANBICKIS & I. LACE
Environment Modelling Centre, Riga Technical University, 1/4 Meza Street, Riga, LV-1048, Latvia
e-mail: emc@egle.cs.rtu.lv

Abstract Two validated ideas are proposed for using in MODFLOW. The first idea proposes to apply an elevation map of a ground surface with water bodies (rivers, lakes, etc) included as the piezometric boundary condition on the top of 3-D hydrogeological model (HM). In such a regime HM automatically computes an infiltration flow distribution. The second idea offers to use a shell of HM as an interpolator for computing boundary conditions when the shell intersects with areas of hydrogeological windows.
Key words hydrogeological models; boundary conditions, infiltration flow

INTRODUCTION

To describe our results, the mathematics of semi-3-D steady state HM, describing mean annual conditions, must be introduced. The *xyz*-grid of HM is built using ($h\times h\times m$)-sized blocks (h is the block plane size; m is a variable block height). The blocks constitute a rectangular *xy*-layer system. Its four vertical sides compose the shell of HM. The ground surface ψ_{rel} and the lower side of the model are its geometrical top and bottom, accordingly. In HM, the vector φ of the piezometric head is approximated, in nodes of the 3-D grid of HM, by the following algebraic equation system:

$$A\ \varphi = b, \quad A = A_{xy} + A_z - G, \quad \beta = \beta_{in} + \beta_{bot} + \beta_{sh} + \beta_w\,, \quad \beta_\psi = G\ (\psi - \varphi) \tag{1}$$

where the matrices A_{xy}, A_z, G represent, correspondingly, the horizontal links (arranged in *xy*-planes) of aquifers, the vertical ties originated by aquitards, the elements connecting nodes of the grid with the piezometric boundary conditions ψ; the vector β accounts for boundary flows: β_w is the water production rate in wells; β_{in}, β_{bot} and β_{sh} are the boundary surface flows, which may be specified on the top, bottom, and shell areas of HM, respectively; β_ψ is the computed flow passing through elements of G.

The flows β_{in}, β_{bot} and β_{sh} can hardly be obtained from field data. By using ψ_{rel}, ψ_{bot}, ψ_{sh}, respectively, all three flows can be changed for the more exact ones of the β_ψ-type (Spalvins *et al.*, 2000). This paper explains how $\beta_{in} \rightarrow \beta_{\psi\, in}$ is performed for the infiltration flow β_{in}, which dominates (1) in regional HM. It is also shown how the shell of HM can be used as an interpolator for the boundary conditions ψ_{sh}. Both methods are helpful for users of the MODFLOW system.

MODELLING OF INFILTRATION

Customary, the infiltration flow is applied on the top surface of fine local scale HM, as an independent constant β_{in}, for recharge areas of the first unconfined quaternary aquifer q. Unfortunately, this simple method fails when crude regional HM for large territories should be formed:

- β_{in} should be variable both for recharge and discharge areas, because the surface elevations ψ_{rel} and ascending flows also vary, respectively;

- for recharge areas, even small errors of β_{in} (x,y) may result in dramatic failures of the computed groundwater table φ_q, as part of φ for (1).

The stability problem caused by β_{in} can be revealed by considering the ratio β_{in} / β_q (β_q - lateral flow) as a function of h for a grid block ($h \times h \times h_q$). To estimate the ratio, some typical parametres may be used: $\beta_{in} = h^2 \times 10^{-3}$ m^3 day^{-1}, $\beta_q = h\, h_q\, k_q\, I_q$ where $h_q = 10$ m, $k_q = 10$ m day^{-1} and $I_q = 0.005$ are the thickness, permeability and hydraulic gradient of the q-block, respectively. Then $\beta_q = h \times 10 \times 10 \times 0.005 = 0.5\, h$ and $\beta_{in} / \beta_q = 2\, h \times 10^{-3}$. For regional HM, $h = 500$ m - 5000 m and $\beta_{in} / \beta_q = 1$ - 10, correspondingly. Because $\beta_{in} \geq \beta_q$, results of HM depends mostly on β_{in}.

The team of the Environment Modelling Centre (EMC) of the Riga Technical University had met with the problem caused by β_{in} and solved it when regional HM for the central part of Latvia was created (Spalvins *et al.*, 1995).

For discharge areas caused mostly by rivers and lakes, the customary method was used for settling discharge flows $\beta_{\psi in}$, as part of (1):

$$\beta_{\psi in} = G_{aer} \left(\psi_{rel} - \varphi_q \right), \quad g_{aer} = h^2\, k_{aer} / h_{aer} \tag{2}$$

where G_{aer} (submatrix of G) contained conductances g_{aer} of river and (or) lake beds representing the saturated aeration zone. These conductances were vertical ties connecting the grid nodes of φ_q and ψ_{rel} planes of HM.

To prevent the instability caused by β_{in}, the EMC team applied (2) for the whole top surface of HM. Then, for recharge areas, g_{aer} supported descending $\beta_{\psi in}$. This idea was mentioned by Bear (1979), but not applied for modern HM. Formerly, g_{aer} was used for modelling infiltration on analog models (Luckner & Schestakow, 1976).

If ψ_{rel} is used as a boundary condition then no instability due to infiltration arises, because, unlike β_{in}, $\beta_{\psi in}$ given by (2) is a dependent parameter. The above innovation has provided the following useful results if humid territories are considered:

- boundaries between the recharge and discharge areas ($\beta_{\psi in} = 0$) may be obtained; they appear even for a steep hillside where groundwater usually seeps out from its footing;
- for recharge areas, φ_q roughly follows $\psi_{rel} > \varphi_q$;
- like observed in nature, maximal recharge values of $\beta_{\psi in}$ appear for heights of the ground surface;
- if a groundwater withdrawal causes lowering of φ_q then $\beta_{\psi in}$ increases there.

None of the above features are reachable automatically if infiltration is modelled by β_{in} as an independent flow.

Thicknesses h_{aer} and m_q of the aquifer q and the zone aer are, as follows:

$$m_q = h_{aer} + h_q, \quad h_{aer} = \delta = \psi_{rel} - \varphi_q, \quad \text{if } \delta \geq 0, \quad h_{aer} = \Delta_{aer} > 0 \quad \text{if } \delta < 0 \tag{3}$$

where Δ_{aer} is the thickness of the discharge area. The real values of $h_{aer} = \Delta_{aer}$ and k_{aer} are difficult to obtain even from field data. For this reason, one may apply conditionally small $\Delta_{aer} = \Delta =$ const and to adjust values $g_{aer} = h^2\, k_{aer} / \Delta$ by altering k_{aer}. As calibration targets for g_{aer}, discharge flows $\beta_{\psi in}$ of (2) should be used. For the sake of simplicity, it is assumed here that the aquifer q does not get dewatered. For real cases, not only the aquifer q, but also lower neighboring layers can be part of h_{aer}. This difficulty occurred when regional HM for the Noginsk region, Russia was formed (Spalvins, 2002).

Initially, the distribution h_{aer} for the recharge areas and location of their borderlines are unknown. Fortunately, some data about a mean thickness $h_{aer\,m}$ of the zone *aer* may be available. Then, as an initial crude assumption, one can fix $g^{(0)}_{aer} = h^2\, k_{aer\,m} / h_{aer\,m}$ = const, for all nodes of the recharge areas ($k_{aer\,m}$ - the mean value of k_{aer}). From the above numerical example, $k_{aer\,m} = 10^{-3}$ m day^{-1}.

To simplify iterative calibration of (h_q, h_{aer}) and $\beta_{\psi\,in}$, in the MODFLOW environment, the EMC team uses, as the first guess, $h_{aer} = \Delta = \Delta_{aer} = 0.02$ m elsewhere on the top surface of HM. A fictitious extra aquifer *rel* of the thickness Δ should be introduced to apply the surface ψ_{rel}, as the boundary condition (any $k_{rel} > 0$ may be used here). The value of $\Delta = 0.02$m has been chosen arbitrary. It must be small enough not to disturb the HM geometry and to provide automatically proper values of elements for A_{xy} and A_z when some layers, included in HM, are discontinuous ($m = 0$).

To prevent triggering of MODFLOW automatics for unconfined and discontinuous layers, all aquifers of HM must be used as confined. The aeration zone *aer* should be treated as a formal aquitard.

The initial permeability base map $k^{(0)}_a$ of the zone *aer* contains the following distinct mean values: $k^{(0)}_a = 10^{-3}$ and 1.0, respectively, for the expected recharge areas and for lines (or areas) of the hydrographical network. This map is used to compute initial values of $g^{(0)}_{aer}$:

$$g^{(0)}_{aer} = h^2\, k^{(0)}_{aer} / \Delta, \quad k^{(0)}_{aer} = c_{aer}\, k^{(0)}_{a}, \quad c_{aer} = \Delta / h_{aer\,m} \tag{4}$$

where c_{aer} accounts for $h_{aer\,m} \rightarrow \Delta$. If $\Delta = 0.02$ m and $h_{aer\,m} = 2.0$ m then $c_{aer} = 10^{-2}$.

For the transmissivity of the aquifer q, the initial values $a^{(0)}_q$ are as follows:

$$a^{(0)}_q = k^{(0)}_q\, m_q\,, \quad k^{(0)}_q = c^{(0)}_q\, k_q, \quad c^{(0)}_q = (m_q - \Delta) / m_q \sim 1.0. \tag{5}$$

When $g^{(0)}_{aer}$ and $a^{(0)}_q$ have been applied, the values of $\varphi^{(0)}_q$ can be obtained. Then:

$$h^{(1)}_{aer} = \delta^{(1)} = \psi_{rel} - \varphi^{(0)}_q, \quad \text{if } \delta^{(1)} \geq \Delta; \quad h^{(1)}_{aer} = \Delta, \quad \text{if } \delta^{(1)} < 0; \tag{6}$$
$$a^{(1)}_q = k^{(1)}_q\, m_q\,, \quad k^{(1)}_q = c^{(1)}_q\, k_q, \quad c^{(1)}_q = (m_q - h^{(1)}_{aer}) / m_q.$$

By using (6), values of $h^{(1)}_{aer}$ can be obtained and the improved map of $k^{(1)}_q$ prepared. Available estimates of β_{in} and h_{aer} must be used as targets for calibration, performed in accordance with (4), (5), (6). Only few iterations are needed to achieve acceptable results for recharge areas. The fictitious thicknesses $h_{aer} = \Delta$, $h_q = m_q$ may be kept until the final $\varphi^{(t)}_q$ is obtained. During iterations $i = 1, 2, \ldots, t$, only $k^{(i)}_{aer}$ and $k^{(i)}_q$ vary. If necessary, the real geometry h_{aer}, $h_q = m_q - h_{aer}$ and the permeabilities k_{aer}, k_q can be introduced. Then $k_{aer} = k^{(t)}_{aer}\, h_{aer} / \Delta$ should be applied.

For the recharge areas, the above algorithm is based on the assumption: g_{aer} = const. Necessary deviations from this rule should be formed on the map $k^{(i)}_a$. The following more universal algorithm (Spalvins, 2002) has been applied, to simplify iterative adjustment of $k^{(i)}_{aer} = c^{(i)}_{aer}\, k^{(i)}_a$:

$$c^{(i)}_{aer} = c^{1-u}_{aer} (\Delta / h^{(i)}_{aer})^u, \quad \text{if } h^{(i)}_{aer} > h_{aer\,m},$$
$$c^{(i)}_{aer} = c_{aer}, \qquad \text{if } h^{(i)}_{aer} \leq h_{aer\,m} \tag{7}$$

where the parametre $h_{aer\,m}$ not only presents a real feature of the zone *aer*, but it also may serve as a formal factor to control the algorithm of (7); the power u ($1 \geq u \geq 0$) is used to vary $k^{(i)}_{aer}$ for recharge areas. The value $u = 0$ represents the considered above initial choice: c_{aer} = const $\rightarrow$ g_{aer} = const. If $u = 1$ then $\beta_{\psi\,in}$ = const where $h_{aer} > h_{aer\,m}$.

The area of constant $\beta_{\psi\, in}$ may be enlarged if a small value of $h_{aer\, m}$ is applied. This version describes the other extremity of the recharge model. Theoretically, the right distribution of $\beta_{\psi\, in}$, for the recharge areas, should be sited somewhere between the ones, provided by the values $u = 0$ or 1, respectively. It has been found experimentally that c = 0.75 is a good choice for most of practical cases (Spalvins, 2002).

BOUNDARY SHELLS AS INTERPOLATORS

Special problems arise when a vertical hydraulic gradient between interlinked layers becomes very small. It happens within hydrogeological windows ($m = 0$) i.e. discontinuous aquitards where elements a_z of A_z are very large (theoretically, $a_z \rightarrow \infty$ if $m = 0$). The EMC team uses $\Delta = 0.02$ m instead of $m = 0$ and then, within the body of HM, solution φ can be found even in complex cases (Spalvins *et al*., 1995), when non-existent fragments of aquitards are part of a multi-tiered system where aquifers may be also absent ($a_{xy} = 0$ of A_{xy}).

If on the shell of HM the condition ψ_{sh} is used and the shell intersects with the non-existent layers then, due to smallness of the vertical hydraulic gradient there, no modeller can settle ψ_{sh} on such intersections. The missing parts of ψ_{sh} can be obtained automatically if the shell acts as an interpolator. The elements $(g_{xy}, g_z)_{sh}$, as part of G, represent all features of geological strata intersected by the shell. To convert the shell into the interpolator, a multiplier constant $u_{sh} = 10^3 - 10^5$ is introduced. It enlarges artificially the values $(g_{xy}, g_z)_{sh}$ of the links connecting nodes of the shell. The converted shell then interpolates missing values of φ_{sh}, as part of the solution φ, at nodes where no initial boundary ψ - condition is fixed (Spalvins, 2002).

The converted shell enables the creation of HM of considerable complexity. This useful approach can be used in all kinds of modelling programs, MODFLOW included.

CONCLUSIONS

Helpful ideas for users of MODFLOW have been developed by the EMC team:

- infiltration flows for recharge areas of HM can be obtained automatically if the ground surface elevation map is applied as the piezometric boundary condition; this method is tested for humid territories.
- the shell of HM may be changed into an interpolator providing missing parts of boundary conditions where the shell crosses with discontinuous geological layers.

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