Ground surface elevation maps as essential boundary condition in reliable hydrogeological models

A.Spalvins
Environment Modelling Centre, Riga Technical University, Latvia

ABSTRACT: The team of the Environment Modelling Centre (EMC) of the Riga Technical University has developed an effective method incorporating the ground surface elevation map, as a boundary condition of a three-dimensional (3D) hydrogeological model (HM). Due to this handy application, reliability of any HM improves considerably.

1 INTRODUCTION

To narrow our study, only semi-3D steady state HM, describing mean annual conditions, is considered. The *xyz*-grid of HM is built of ($h*h*h_z$)-sized blocks (h is the block plane size; h_z is a variable block height). They constitute a rectangular *xy*-layer system. Its four vertical sides compose the shell of HM. The ground surface *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 sought, in nodes of the 3D grid of HM, as the solution of the following algebraic equation system:

$$A\ \varphi = \beta - G\ \psi,\quad A = A_{xy} + A_z - G,$$

$$\beta = \beta_{in} + \beta_{bot} + \beta_{sh} + \beta_w,\quad \beta_\psi = G\ (\psi - \varphi) \qquad (1)$$

where the matrices A_{xy}, A_z, and G represent, correspondingly, the horizontal links a_{xy} of aquifers, the vertical ties a_z originated by aquitards, and the elements g_{xy}, g_z that are connecting nodes of the grid with the piezometric boundary conditions ψ; the vector β accounts for the fixed boundary flows: β_w is the given 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, correspondingly; β_ψ is the computed flow passing through elements of G.

Unluckily, true distributions of the flows β_{in}, β_{bot} and β_{sh} can hardly be obtained from field data. Crude substitutes of these fixed flows inevitably produce bad HM results. Fortunately, all three flows can be changed for the more exact ones of the β_ψ-type (Spalvins et al. 2000). This paper explains how the transformation $\beta_{in} \rightarrow \beta_{\psi\ in}$ should be performed for the infiltration flow β_{in}. For HM of humid areas, the infiltration is the weightiest boundary condition of (1). For this reason, appliance of $\beta_{\psi\ in}$ always results in considerable improvement of HM.

2 THE GROUND SURFACE ELEVATION MAP AS THE BOUNDARY CONDITION

Since 1995, the EMC team has successfully applied (Spalvins et al. 1995) the ground surface elevation map ψ_{rel}, as the ψ-type boundary condition. This method assumes that the aeration zone *aer* (unsaturated part of the unconfined q aquifer) behaves like an aquitard that contains areas of descending (recharge) and ascending (discharge) infiltration flows. The ascending flows are caused mostly by the hydrographical network (rivers, lakes, etc.).

The permeability k_{aer} of the *aer* zone can be apprised by applying the mean annual relative permeability k_{rm}:

$$k_{rm} = h_{aer} / \int_0^{h_{aer}} k_r^{-1} dh_c\ ,\quad k_{aer} = k_{rm}\, k_q \qquad (2)$$

and the van Genuchten's (vG) capillary model (3) for any unsaturated soil (Genuchten 1980). In (2), $0 \le k_r \le 1$ is the current relative permeability; h_{aer} is the thickness of the zone $0 \le h_c \le h_{aer}$; k_q is the permeability of the q aquifer. Just below the ground surface of the recharge areas, k_r diminishes due both to evaporation processes and an impact of the capillary curve $s = s(h_c)$ there; $0 \le s \le 1$ is the normalized soil water content. The following formula:

$$k_r = s^{0.5}(1-(1-s^{1/m})^m)^2,\quad s = (1 + (\alpha h_c)^{1/(1-m)})^{-m} \qquad (3)$$

enables to estimate k_r. In (3), the relationship $s = s(h_c)$ is the kernel of the vG model, where the parametres α and m are used for its controlling. If

$s \sim 1$ then $k_r \sim 1$ (discharge areas); in the recharge areas: $s << 1$, k_r is small, and the *aer* zone behaves like an aquitard if its mean annual state is considered.

When ψ_{rel} is applied, the flow $\beta_{\psi\ in}$ passes through the aeration zone:

$$\beta_{\psi\, in} = G_{aer}\ (\psi_{rel} - \varphi_q), \quad g_{aer} = k_{aer}\, h^2 / h_{aer} \geq 0 \qquad (4)$$

where φ_q is the computed head (subvector of φ) for the q aquifer; G_{aer} (diagonal submatrix of G) contains the vertical ties g_{aer} connecting ψ_{rel} with φ_q. The expression (4) reflects the usual support of HM when the ψ-condition is applied. The $\beta_{\psi\ in}$ distribution is also handy for the HM calibration - both, as its tool (g_{aer} variable) and target (some observed data for β_{in} and φ_q are available). The calibrated $\beta_{\psi\ in}$ must be obtained iteratively under the following rule used by EMC, "due to complexity of any geometrical change of HM, the geometry must remain fixed, until the final calibrated φ-distribution is obtained". In reality, h_{aer} is variable:

$$\text{if} \quad \beta_{\psi\, in} \geq 0, \quad h_{aer} = \psi_{rel} - z_q - h_q, \quad h_q = \varphi_q - z_q;$$

$$\text{if} \quad \beta_{\psi\, in} < 0, \quad h_{aer} = \Delta = 2 \text{ cm} \qquad (5)$$

where z_q and h_q are, correspondingly, the bottom elevation surface and the water saturated thickness of the unconfined q aquifer. For the discharge areas ($\beta_{\psi\ in} < 0$), nearly no field data regarding h_{aer} are available. For this reason, we conditionally assume $h_{aer} = \Delta$. Fictitious Δ is applied by the EMC team also for other purpose (see below).

As it follows from (5), real h_{aer} and h_q are unknown beforehand and should be obtained, as the by-products of the calibrated system of (1). Fortunately, there is no actual need to follow the real geometry (5), in order to obtain the calibrated φ-distribution. However, the geometry is important if HM is applied as a driver for modelling contaminant transport processes in groundwater. The methodology of EMC enables to account for the real geometry of HM, if necessary.

In HM, the q aquifer should be conditionally confined, and the initial try for its transmitivity distribution a_q is, as follows:

$$a_q^{(0)} = c_q^{(0)}\, k_q^{(0)}\, h_q^{(0)}, \quad h_q^{(0)} = \psi_{rel} - z_q + \Delta \qquad (6)$$

where $c_q^{(0)}$, $k_q^{(0)}$, and $h_q^{(0)}$ are the initial distributions (represented by diagonal matrices), correspondingly, of the correction factor (dimensionless), the permeability, and the thickness for the q aquifer; the constant Δ is used if q is discontinuous (in some areas, $\psi_{rel} - z_q = 0$); $h_q^{(0)}$ is the full thickness of the q aquifer; until HM has not been calibrated, $h_q^{(0)}$ remains unchanged. The exact value of the factor c_q is:

$$c_q = (h_q^{(0)} - h_{aer}) / h_q^{(0)} = var \leq 1.0\,. \qquad (7)$$

Hence $h_{aer}^{(0)} = \Delta$ (see (8)) then $c_q^{(0)} = 1.0$. The constant Δ is used for all kinds of discontinuous or fictitious layers of HM. Due to smallness of Δ, the HM geometry is not really distorted, even if numerous layers of such kind are involved. For their non-existent parts, Δ serves the following tasks:

- controls values of elements a_{xy} (a_q of (6)) and a_z (g_{aer} of (4)) via the proper choice of the corresponding permeability k_{xy} (k_q of (6)) and k_z (k_{aer} of (4)) distributions;
- prevents an occurrence of a negative thickness for a layer, due to computational round off errors of its top and bottom surfaces (ψ_{rel} and z_q for (6)).

The value of Δ may be chosen rather arbitrary. It must be small enough not to disturb the HM geometry of multilayered systems and also to cause large values of the elements a_z, for the non-existent parts of discontinuous aquitards.

For $g_{aer}^{(0)}$, the general formula (4) must be specified, because instead of the unknown variable h_{aer}, constant $h_{aer}^{(0)} = \Delta$ should be applied temporarily elsewhere:

$$g_{aer}^{(0)} = c_{aer}^{(0)}\, k_{aer}^{(0)}\, h^2 / \Delta, \quad c_{aer}^{(0)} = \Delta / h_{aerm} \qquad (8)$$

where the roles of $c_{aer}^{(0)}$, $k_{aer}^{(0)}$ are the same, as for the q aquifer; $h_{aer\ m}$ is the mean thickness of the recharge area for the *aer* zone. Until $\beta_{\psi\ in}$ has not been calibrated, $h_{aer}^{(0)} = \Delta$.

The $k_{aer}^{(0)}$-distribution contains the following distinct mean values: $k_{aer} \sim 10^{-3}$ and 1.0, correspondingly, for the recharge areas and for the lines (or areas) of the hydrographical network. If $h_{aer\ m} \sim 2$ metres then $c_{aer}^{(0)} \sim 10^{-2}$.

When the initial distributions (6) and (8) are applied, HM usually provides good results:

- the surface $\varphi_q^{(0)}$ automatically follows main geometrical features of ψ_{rel}, because g_{aer} interlinks both surfaces; for humid areas, this natural phenomenon always takes place;
- it follows from (4) that components of $\beta_{\psi\ in}$ respond correctly to a depression cone caused by the β_w flow ($\beta_{\psi\ in}$ increases if the cone gets deeper); when fixed β_{in} is used, this important natural response cannot be automatically accounted for by HM;
- for a modeller, HM provides the $\beta_{\psi\ in}^{(0)}$ distribution; it informs about the infiltration intensity and clearly indicates areas of discharge and recharge;
- convergence of any iterative solution method of (1) improves considerably, because, on the HM top surface, the piezometric boundary condition ψ_{rel} is applied instead of β_{in}.

Any complex distribution $\beta_{\psi\ in}$ can be controlled rather simply via the change of k_{aer}:

- for the recharge areas, the right k_{aer} distribution is found if the computed groundwater table φ_q matches the observed one, and $\beta_{\psi\ in}$ does not differ considerably from the expected mean infiltration values;

- for the discharge areas, k_{aer} must provide the estimated flow and evaporation rates, respectively, for running (rivers, ditches…) and standing (lakes, pools…) surface water sources; to obtain g_{aer} of (4), there is no attempt made to use any of the practically unknown parametres (width / thickness, permeability) of the water source bed, which are conventionally recommended by (McDonald & Harbaugh 1988), because it is enough to search for k_{aer} only.

Therefore, the calibration of the flow $\beta_{\psi\ in}$ is performed mainly by adjusting the k_{aer} map. Minor settlements of this flow may be achieved also due to some adjustment of k_q.

It follows from the above comments about calibration of $\beta_{\psi\ in}$ that the ψ_{rel}-map enables to integrate all kinds of HM natural boundary conditions, applied on its top surface.

The advantage of $\beta_{\psi\ in}$ (predicted by HM as a part of (1)) over conventional fixed β_{in} (quessworked by a modeller) is considerable, because $\beta_{\psi\ in}$ is based on reliable initial data. They are carried mostly by ψ_{rel} and the system of (1), as a whole.

In practice, even the crude attempt (6) and (8) provides surprisingly good results for complex regional HM (Spalvins et al. 1996, Gosk et al. 1999). In these cases, likely, no HM can be obtained if the conventional approach of fixed β_{in} is applied. The reasons for such a pessimism are, as follows:

- for regional HM, the infiltration distribution is very complex, because it should account for numerous recharge and discharge areas;
- if 3D regional HM contains many geological layers then it is nearly impossible to predict the reaction of the HM body on the fixed β_{in} flow: the computed watertable φ_q often occurs high above the ground surface ψ_{rel} (an impossible situation for an unconfined aquifer), because φ_q does not follow ψ_{rel} if infiltration β_{in} is fixed.

For both above HM, no restoration of the real geometry was accomplished, because mass transport modelling was not performed at the research stage reported. However, the real geometry can be obtained, if necessary (see the next section).

The method of modelling the mean annual infiltration can be run by any HM system, for example, by the Groundwater Vistas program (Environmental Simulations 1997). However, no regimes of unconfined aquifers must be used there, otherwise the MODFLOW code involved may ruin HM, especially, if HM contains discontinuous layers (McDonald & Harbaugh 1988). Then the destruction of HM is inevitable, due to irreparable, automatic annihilation of "dried" ($h_q = 0$) cells. This cannot be prevented for the non-existent areas of discontinuous aquifers, because their thickness is zero, as the geometrical feature.

To immerse the ψ_{rel}-map, in the MODFLOW code environment, the surface *rel* should be specified, as a formal thin aquifer ($\Delta_{rel} = 2$ cm).

Recently an advanced version for the flow $\beta_{\psi\ in}$ simulation has been developed and tested (Spalvins 2000a, Spalvins 2000b). The version is described below.

3 AN ADVANCED VERSION OF INFILTRATION SIMULATION

The formula of (8) does not include any information, but h_{aerm}, about real h_{aer}. Instead of h_{aer}, small Δ is used throughout the calibration process of $\beta_{\psi\ in}$. Such an approach is based on the following motives:

- if $h_{aer}^{(0)} = \Delta$, the number of variable factors in g_{aer} is minimal and only the right k_{aer}-distribution should be found, because the constant $c_{aer}^{(0)}$ is chosen to provide the reasonable first results only;
- the transformation $h_{aer}^{(0)} \rightarrow h_{aer}$ has no real influence on the calibrated flow $\beta_{\psi\ in}$;
- for the recharge areas, the values of k_{aer} are rather independent from h_{aer}, because just smallest k_r, from the "ground-air" interface, mainly determine k_{rm} of (2).

It was noticed recently (Spalvins 2000b) that the statement about the weak relationship between k_{aer} and h_{aer} should be corrected, if $h_{aer} > h_{aerm}$. This idea caused further development of the method of modelling $\beta_{\psi\ in}$.

After the initial rough calibration of HM ($k_q^{(0)} \rightarrow k_q^{(1)}$; $k_{aer}^{(0)} \rightarrow k_{aer}^{(1)}$), the solution $\varphi_q^{(1)}$ is obtained, and improved distributions $h_{aer}^{(1)}$ and $h_q^{(1)}$ can be specified:

$$h_q^{(1)} = h_q^{(0)} - h_{aer}^{(1)} + \Delta\,, \tag{9}$$

$$h_{aer}^{(1)} = \begin{cases} \delta^{(1)} = \psi_{rel} - \varphi_q^{(1)} & \text{if } \delta^{(1)} > \Delta\,, \\ \Delta & \text{if } \delta^{(1)} \le \Delta\,, \end{cases} \tag{10}$$

In (9), $\delta^{(1)} \le \Delta$ holds mostly for the discharge areas. If real h_{aer} is unknown then $h_{aer}^{(1)} = \Delta$ here.

Hence the distributions $h_{aer}^{(1)}$, $h_q^{(1)}$ still cannot be applied directly (HM geometry fixed temporarily!), the correction factors $c_q^{(1)}$, $c_{aer}^{(1)}$ must be computed:

$$c_q^{(1)} = h_q^{(1)} / h_q^{(0)}, \tag{11}$$

$$c_{aer}^{(1)} = \begin{cases} \sigma^{(1)} = (\Delta / h_{aer}^{(1)})^u & \text{if } h_{aer}^{(1)} > h_{aerm}, \\ c_{aer}^{(0)} & \text{if } h_{aer}^{(1)} \le h_{aerm} \end{cases} \tag{12}$$

where $1 > u > 0$ is the parametre used to control $c_{aer}^{(1)}$ for the recharge areas if $h_{aer}^{(1)} > h_{aerm}$. Currently, $u = 0.75$ has been accepted as an optimal choice. For the recharge areas, the rule (12) reduces $\beta_{\psi\ in}$ if $h_{aer}^{(1)} > h_{aerm}$. Then $\sigma^{(1)}$ is variable.

The factors $c_q^{(1)}$, $c_{aer}^{(1)}$ must be applied for the current approximation of a_q and g_{aer} :

$$a_q^{(1)} = c_q^{(1)}\, k_q^{(1)}\, h_q^{(0)},\;\; g_{aer}^{(1)} = c_{aer}^{(1)}\, k_{aer}^{(1)}\, h^2 / \Delta. \quad (13)$$

The HM further calibration provides final values $h_q^{(1)} \rightarrow h_q^{(i)}$ and $h_{aer}^{(1)} \rightarrow h_{aer}^{(i)}$ of (9) and (10), accordingly. The distributions $a_q^{(1)} \rightarrow a_q^{(i)}$ and $g_{aer}^{(1)} \rightarrow g_{aer}^{(i)}$ are also obtained.

If necessary, the real HM geometry can be introduced now, instead of the fixed one. This action has no impact on numerical values of $a_q^{(i)}$ and $g_{aer}^{(i)}$. It replaces only their formal ingredients, as follows:

$$a_q^{(i)} = k_q^{(i)}\, h_q^{(i)},\;\; g_{aer}^{(i)} = k_a^{(i)}\, h^2 / h_{aer}^{(i)},$$

$$k_a^{(i)} = c_{aer}^{(i)}\, k_{aer}^{(i)}\, h_{aer}^{(i)} / \Delta \quad (14)$$

where $h_q^{(0)} \rightarrow h_q^{(i)}$, $\Delta \rightarrow h_{aer}^{(i)}$, and $k_{aer}^{(1)} \rightarrow k_a^{(i)}$. Now from (5), one can obtain final z_q that is applied as an input for the Groundwater Vistas system.

4 CONCLUSIONS

For humid areas, the infiltration flow is the dominant HM boundary condition. Unfortunately, for complex regional cases, the conventional way of using fixed infiltration flows cannot provide good results.

The EMC team has developed and proved the new method of obtaining this weighty boundary flow via using the ground surface elevation map, as the reliable boundary condition. The method can be run by any modelling system related to creating of HM.

Reliability of HM results has increased drastically, even for the case, when the robust form of the new method is applied.

REFERENCES

Spalvins, A., Slangens, J., Janbickis, R., Lace, I. & Gosk, E. 2000. Methods for Improving Verity of Groundwater Modelling. *Proc. of 16th IMACS World Congress, Lausanne, Switzerland, 21-25 August 2000.* 6 pages on CD-ROM, ISBN 3-9522075-1-9.

Van Genuchten, M.Th. 1980. A closed - form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Amer. J. (44): 892-898.

Spalvins, A., Janbickis, R., Slangens, J., Gosk, E., Lace, I., Viksne, Z., Atruskievics, J., Levina, N. & Tolstovs, J. 1996. Hydrogeological Model "Large Riga". Atlas of maps. Riga – Copenhagen: (*Boundary Field Problems and Computers, 37th issue*).

Environmental Simulations, Inc. 1997. Groundwater Vistas. Guide to using.

Gosk, E., Spalvins, A., Vartanyan, G. (eds.). 1999. Hydrogeological and contamination transport models for Noginsk district, Moscow region. *Report on sub-contractor agreement within the project: "Groundwater contamination and remediation in Noginsk district, Moscow region",* Riga - Moscow.

Spalvins, A., Janbickis, R. Slangens, J., Gosk, E., Lace, I., Viksne, Z., Atruskievics, J., Levina, N. & Tolstovs, J. 1996. Development of Regional Hydrogeological Model "Large Riga". *Proc. of International Seminar on "Environment Modelling".* Riga – Copenhagen,1995. Vol.1. - p.145-158 (*Boundary Field Problems and Computers, 36th issue*).

Spalvins, A. 2000a. Landscape Elevation Maps as Reliable Boundary Condition for Hydrogeological Models. *Scientific Proceedings of Riga Technical University in series "Computer Science".* Riga. (*Boundary Field Problems and Computer Simulation, 42nd issue).*

McDonald, M., & Harbaugh, A. 1988. A modular three-dimensional finite-difference groundwater flow model. U.S. Geological Survey. Open files report 83-875. Washington.