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Boundary shells of hydrogeological models as interpolation devices

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ABSTRACT: For complex hydrogeological models (HM) including areas of non-existent geological structures, it is difficult to specify boundary conditions on the HM shell. These conditions can be obtained automatically when the shell of HM is used, as a special interpolation device.

1 INTRODUCTION

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 (in the *xy*-space) layer system approximating a set of geological structures (aquifers and aquitards). Four vertical sides of HM compose its shell. The landscape surface and the lower side of HM are its geometrical top and bottom, respectively. According to the methodology developed by the Environment Modelling Centre (EMC) of the Riga Technical University (Spalvins et al., 2000), a reliable piezometric boundary ψ–distribution can be applied, on the whole surface of HM, in order to ensure high quality of simulation results. However, some difficulties of interpolating this distribution, on the HM shell, arise if HM includes geological structures containing non-existent parts (absent areas of aquifers and “windows” of aquitards). This paper describes an original numerical method removing this kind of interpolation difficulty.

To understand the problem, some mathematics is needful. The vector φ of the piezometric head is the numerical solution provided, in nodes of the HM grid, by the following algebraic equation system:

$$A\,\varphi = \beta - G\,\psi, \quad A = A_{xy} + A_z - G, \tag{1}$$

where β is the source vector representing pumping rates of wells; G is the diagonal matrix composed of elements connected to boundary nodes where ψ values are given; the matrices A_{xy}, A_z, contain, correspondingly, horizontal links a_{xy} between adjacent grid nodes of aquifers and vertical ties a_z (originated by aquitards) connecting adjoining aquifers; G also contains elements g_{xy}, g_z of a similar origin. For the above described semi-3D scheme, the values of elements a_{xy}, a_z (or g_{xy}, g_z) are computed, as follows:

$$a_{xy} = k\,h_z, \quad a_z = h^2\,k\,/\,h_z\,, \tag{2}$$

where h_z, k are, accordingly, elements of h_z, k–maps of computed thickness and permeability distributions of geological layers, in nodes of the HM grid.

Some uncertainty of the ψ–distribution, on the HM shell, occurs when the difference between computed φ values, belonging to interlinked aquifers becomes very small. It happens, in areas of hydrogeological windows ($h_z = 0$) of discontinuous aquitards, where the elements a_z of (2) have very large values (theoretically, $a_z \rightarrow \infty$ if $h_z = 0$), and the gradient of φ must be wee here. On an intersection of the window with the shell, the ψ-values behave similarly, as the ones of φ. In complex practical cases, for example (Janbickis et al., 1995), the non-existent parts of aquitards constitute a multi-tiered system where aquifers are also absent ($a_{xy} = 0$). It was necessary to find a method providing a reliable ψ–distribution for the above reported case when numerous places, on the HM shell, possessed almost nil vertical gradients of ψ. Because the areas where the vertical gradients of φ and $\psi \approx 0$ do not disturb space continuity of HM, the method sought must also preserve this fundamental feature.

2 THE SHELL AS AN INTERPOLATION DEVICE

It was clear that no modeller could produce manually the above-described conditions on the shell without distorting the HM space continuity. The problem was solved numerically by introducing a multiplier constant $u_{sh} = 10^3 - 10^5$, to enlarge artificially, the values g_{xy}, g_z, of links connecting nodes of the shell. The converted shell acts like an almost ideally conducting shield which compute missing values of ψ, in its nodes where no initial boundary conditions are fixed, as a special portion of the solution φ.

The above innovation has been used by EMC, since 1995 (Spalvins et al., 1995). Nowadays, the following general methodology is applied, to make the ψ-distributions for the HM shells-interpolation devices:

- the vertical hydrogeological cross section of the shell must be available for a modeller; it appreciably indicates places where non-existent parts of geological structures are located and also helps to foresee a general behavior of the ψ-distributions; on the shell;
- by accounting for observed ψ-data, and using the cross section as the master guide, the modeller must specify, by help of the special CRS program(Lace and Spalvins, 2000), a limited set of characteristic points of initial ψ-values for each aquifer; the set will be used by the CRP program (Slangens and Spalvins, 2000) to create the ψ-data line for each allowed interval of the aquifer; non-allowed parts include intersections with non-existent areas of aquifers and /or aquitards; start and end points of the allowed intervals must be exactly denoted, in order to avoid areas of small vertical gradients of ψ;
- the CRP program transforms the CRS data into the vectored line representation providing fixed values of ψ for these nodes of the shell where it is permitted, the remaining nonfixed parts of ψ are computed, in the course of solving (1), due to the interpolation abilities of the converted HM shell.

One should not involve the shell space into any water balance calculations of HM, because flows of the converted shell are u_{sh}-fold larger that the normal ones. It is possible to include the shell into these balances if its normalization is done:

- the final set of ψ from (1) is applied, as the fixed one;
- the normal values of g_{xy}, g_z are used instead of the enlarged ones.

The method of transforming elements of the shell was also applied, in the broader sense than described above, for controlling features of the Geological Data Interpolation (GDI) program (Spalvins and Slangens, 1994). This program is being applied, until now, for obtaining digital 2*D* maps of *k*, h_z and other parametres. The GDI-interpolated surface, for example, the *k*-map of (2) of the *i*-th aquifer plane of (1) presents the numerical solution (in the φ–form) of a special boundary problem stated for *k*, on this grid plane. Only boundary conditions of the ψ–type are used, as pointvise and line initial data. No β–data are allowed to ensure fulfillment of the minimum/maximum principle for results obtained. In GDI, two characteristic district values of the multiplier u_{sh} are mostly applied: $u_{sh} = 0.5$; $u_{sh} \geq 10^4$. As shown before, the larger u_{sh} value turns the rectangular borderline into the device for linear interpolation, between points where initial data are fixed.

If one wants to use a constant boundary value, in all nodes of the shell, this value must be fixed only in one point of the boundary (Spalvins et al., 1995). When nothing is fixed there then some mean boundary value is computed. This original method has been used for creating concentration distributions of contaminants migrating in groundwater (Spalvins, 1998).

If $u_{sh} = 0.5$ then, in fragments where no initial data are specified, the boundary acts like an impervious one (isolines of the interpolated parametre are orthogonal to the shell line). Both characteristic u_{sh} values are applied, because it is very convenient to modify results of the GDI-interpolation in wide range via a trivial change of a single control parameter.

3 CONCLUSIONS

The EMC team has developed an original numerical method allowing use of the converted HM shell for interpolation purposes. This method enables to create HM of utmost complexity because high guilty of boundary conditions, on such a shell, is obtained automatically. This useful novel approach can be applied in all kinds of modelling programs developed for building of HM.

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Spalviņš A., Šlangens J., Janbickis R. Hidroģeoloģisko modeļu robežu čaulas kā interpolejošās ierīces.
Nav viegli definēt robežnoteikumus uz sarežģītu hidroģeoloģisko modeļu (HM) čaulas, ja HM ietver ģeoloģiskos slāņus, kuriem dažas daļas neeksistē. Robežnoteikumus var iegūt automātiski, ja HM čaulu izmanto kā interpolācijas ierīci.

Спалвинь А., Шланген Я., Янбицкий Р. Боковые поверхности гидрогеологических моделей в роли интерполирующих устройств.
Нелегко задать граничные условия на боковой поверхности сложных гидрогеологических моделей (ГМ), если ГМ содержит геологические структуры содержащие несуществующие части. Эти граничные условия можно получить автоматически, если боковая поверхность ГМ, используется в роли интерполирующего устройства.