New subsidiary tools for the modeling system REMO

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ABSTRACT: New subsidiary software tools have been developed for the modeling system REMO. These tools may be used for formulating hydrogeological models (HM) and for computing balance of 3D - groundwater flows.

1 INTRODUCTION

The Environment Modelling Centre (EMC) of the Riga Technical University has developed the modelling system REMO for formulating and running HM (Spalvins et al. 2001). In REMO, numerous subsidiary programs are included which enable to improve results provided by HM. To elucidate the problems solved by the new tools, it is necessary to consider the main mathematical equations of HM.

The *xyz*-grid of HM is built of ($h{*}h{*}\, m$)-sized blocks (h is the block plane size; m is a variable block height). They constitute a rectangular ($2s + 1$) – tiered *xy*-layer system where $s + 1$ and s are, accordingly, the number of aquifers and interjacent aquitards. Its four vertical sides compose the shell of the HM grid. The ground surface (relief) and the lower side of the model are its geometrical top and bottom, respectively.

The vector φ of the piezometric head is the numerical solution of a boundary field problem approximated, 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 the matrices A_{xy}, A_z, and G represent, correspondingly, horizontal links a_{xy} of aquifers (arranged in *xy*-planes), vertical ties a_z originated by aquitards, and elements connecting "free" nodes of the grid with the ones where the piezometric boundary conditions ψ are specified; in REMO, the ψ-distribution exists on the whole HM surface: top + bottom + shell, and the source vector β contains only rates of the groundwater withdrawal via wells. The elements a_{xy}, a_z (or g_{xy}, g_z of G) are computed, as follows:

$$a_{xy} = k\, m, \quad a_z = h^2 k / m, \quad k \geq 0, \quad m_i = h_{zi} = z_{i-1} - z_i \geq 0, \quad i = 1, 2, \ldots, 2s + 1 \tag{2}$$

where z_{i-1} and z_i are the elevation distributions of the top and bottom surfaces of the i-th geological layer; z_0 represents the ground surface map with the hydrograpical network (lakes, rivers, etc.) included; m , k are, accordingly, elements of the digital m, k-maps of computed thickness and permeability distributions of layers. The set of the z_i –maps states the full geometry of HM.

In REMO, various types of data lines (isolines, geological borders and sections, long line profiles of rivers, etc.) may be applied for creating HM. The data line L_σ has its carrier L and the data profile σ. The line L is the broken one passing through the master points $j = 1, 2, \ldots, J$. The set of J - 1 directed straight line segments represents the following vectored form of L:

$$L = \{\ c_j\ \},\ \ j = 1, 2, \ldots, J; \quad l_{1,J} = \sum_{j=1}^{J-1} l_{j,j+1}, \quad l_{j,j+1} = \sqrt{(x_j - x_{j+1})^2 + (y_j - y_{j+1})^2} \tag{3}$$

where $\{\ c_j\ \} = \{\ x_j, y_j\ \}$ is the coordinate set, on the continuos *xy*-plane, of the points where L turns; $l_{1,J}$ and $l_{j,j+1}$ are the lengths, accordingly, of L and the elementary vector linking the adjacent points j and $j + 1$. The shape of σ may be complex, and the additional ponts $k = 1, 2, \ldots, K$ are introduced, to aproximate the curved graph. Then the line L_σ includes $N = J + K$ points (located on L), and L_σ is specified, as follows:

$$L_\sigma = \{ c_i, \sigma_i \}, \quad i = 1, 2, \ldots, N, \quad \{ c_i = c_j \wedge c_k \}, \quad \{ \sigma_i = \sigma_j \wedge \sigma_k \}. \tag{4}$$

The duo sets of the xy-coordinates and the σ-values $\{ c_i, \sigma_i \}$,$\{ c_j, \sigma_j \}$, and $\{ c_k, \sigma_k \}$ represent, accordingly, the current i-th data points, the master wells j of L, and the additional points k dividing the elementary segments $l_{j, j+1}$ of L into collinear pieces.

Special CRP program has been developed (Slangens & Spalvins 2000), to obtain from the initial data the form of (4) and to extract from it the special set $\{ c_s, \sigma_s \}$ where c_s and σ_s are the xy-coordinates and the σ-values, accordingly, at the s-th intersection of L_σ with the grid; this set represents the "c-data" applied for incorporating the lines into HM (Spalvins & Slangens, 1994); the set $\{ c_s, \sigma_s \}$ carries the line L_s, which also approximates L_σ; closeness of these lines depends on the plane step h (finer grid → closer L_s and L_σ).The new software tools apply the set $\{ c_s, \sigma_s \}$ to perform four subsidary tasks explained below.

2 REPLACING HORIZONTAL GRID LINKS

In REMO, the k and m values of (2) is specified in nodes of the HM grid. Let us consider an elementary horizontal link a_{12} connecting two neighbouring nodes 1 and 2. The value of a_{12} is computed, as the mean harmonic:

$$1/ a_{12} = 1/ a_1 + 1/ a_2 , \qquad a_1 = k_1 * m_1, \; a_2 = k_2 * m_2 . \tag{5}$$

The definition (5) imposes severe limitations on values of a_{12}. For example, they cannot by arbitrary. Any a_{12} values can be used if they are specifed individually, in nodes of the finer grid where $0.5h$ step is applied. Then no computations of (5) are necessary. Such a universal approach was used in the first REMO version. In order to make the REMO and MODFLOW systems compatible, the rule (5) is being applied presently.

The new tool partially overcomes the limitations imposed by (5). It replaces any element a_{old} of the a_{xy} type (detected by a line L_a) with the new one a_{new} . The duo set $\{ c_s ,(a_{new})_s \}$ of L_a denotes this operation where the coordinate c_s indicates a_{old} to be replaced. The operation $a_{old} \rightarrow a_{new}$ must also correct these diagonal elements of A_{xy} which incorporate the replaced xy - links.

3 INCORPORATING A DRAIN

A drain d can be specified by a line L_d denoted by the two duo sets $\{ c_s, \psi_s \}$ and $\{ c_s, g_s \}$ where ψ_s and g_s are the values of an elevation and the drain link in the s-th crosspoint, correspondingly.

Joining of d with the grid can be considered for an elementary link a_{12}, where s divides h into the fragments $h_1 + h_2 = h$ (Fig. 1a). If (5) is applied for computing a_{12} then two formal links $a_{1s} = a_{12}\, h / h_1$ and $a_{2s} = a_{12}\, h / h_2$ can be introduced. To join the s-th element of d with the grid, the s-th crosspoint should be eliminated (Fig. 1b):

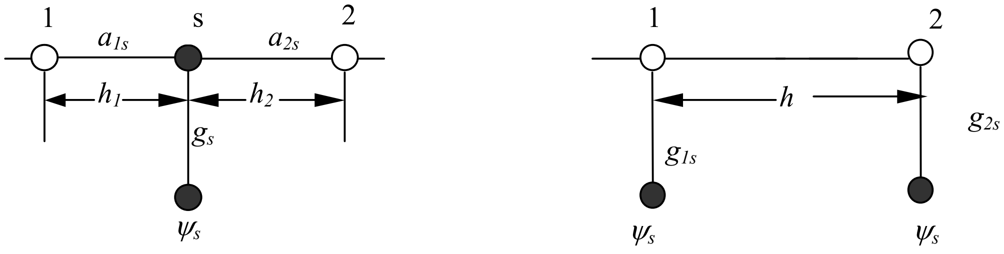
$$(a_{12})_s = a_{1s} * a_{2s} / (a_{1s} + a_{2s} + g_s), \quad g_{1s} = a_{1s} * g_s / (a_{1s} + a_{2s} + g_s) , \quad g_{2s} = a_{2s} * g_s / (a_{1s} + a_{2s} + g_s) \tag{6}$$

where $(a_{12})_s$ and g_{1s} , g_{2s} are values, correspondingly, for the transformed link a_{12} and the two drain links connected to the nodes 1 and 2. Therefore, the elimination replaces $a_{12} \rightarrow (a_{12})_s$, springs up new components for the vector $G\psi$ of (1), and corrects the diagonal elements of A.

Flows I_s for all elements g_s are also provided:

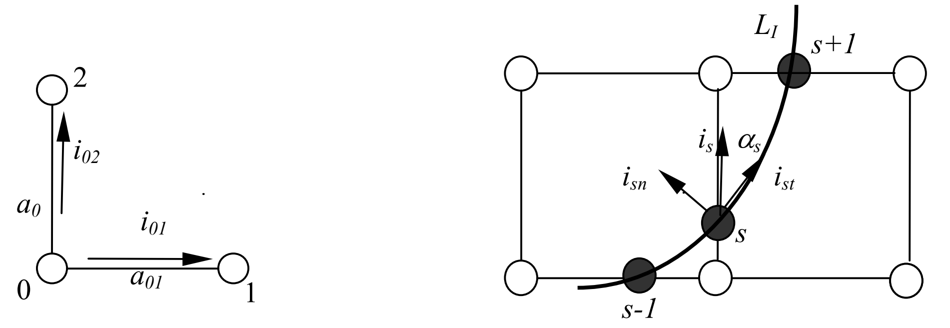
$$I_s = (\varphi_s - \psi_s)\, g_s , \qquad \varphi_s = (\varphi_1 a_{1s} + \varphi_2 a_{2s} + \psi_s g_s) / (a_{1s} + a_{2s} + g_s) \tag{7}$$

where φ_s is the back - interpolated value of φ at the s-th crosspoint. The sum of I_s is also available for the full length of L_d or for any its fragment chosen.



a) before joining b) after joining

Fig. 1. A sheme for joining of an elementary drain with a grid



a) flows i_{01}, i_{02} for x and y links b) normal and tangential flows i_{sn}, i_{st}

Fig. 2. Lateral flows of the grid

4 COMPUTING NORMAL AND TANGENTIAL COMPONENTS FOR THE GROUNDWATER FLOW

In the HM grid, elementary flows i_x and i_y are being computed as vectors for the links $a_x = a_{01x}$, $a_y = a_{02x}$ of A_{xy} (Fig. 2a):

$$i_x = a_{01} (\varphi_1 - \varphi_0) , \qquad i_y = a_{02} (\varphi_2 - \varphi_0) \tag{8}$$

where φ_0, φ_1, φ_2 are heads computed for the nodes *0, 1, 2*. To perform calculations of the groundwater balance, summary normal I_n and mean tangential I_t flows should be computed with respect to the line L_1 specified by its crosspoints $s = 1, 2, \ldots ,N_s$:

$$I_n = \sum_{s=1}^{N_s} i_{sn} , \qquad i_{sn} = i_s \sin \alpha_s , \qquad I_t = N_s^{-1} \sum_{s=1}^{N_s} i_{st} , \qquad i_{st} = i_s \cos \alpha_s \tag{9}$$

where i_s, $i_{sn,}$ and i_{st} are the full normal and tangential flows at the s-th crosspoint accordingly; α_s is the angle formed by L_1 and i_s. The formulas for $\sin \alpha_s$ and $\cos \alpha_s$ depend on i_s given by (8):

$$\begin{aligned} &\sin \alpha_s = (y_s - y_{s+1}) / l_{s,s+1} \quad \text{if } i_s = i_{sx} , && \sin \alpha_s = (x_s - x_{s+1}) / l_{s,s+1} \quad \text{if } i_s = i_{sy} , \\ &\cos \alpha_s = (x_s - x_{s+1}) / l_{s,s+1} \quad \text{if } i_s = i_{sx} , && \sin \alpha_s = (y_s - y_{s+1}) / l_{s,s+1} \quad \text{if } i_s = i_{sy} , \end{aligned} \tag{10}$$

$$l_{s,s+1} = \sqrt{(x_s - x_{s+1})^2 + (y_s - y_{s+1})^2} , \; s = 1, 2, \; ,N_s .$$

If the line L_I coincides with an isoline of φ then $\sin\,\alpha_s = 1.0$ in all crosspoints. On the other hand, $\cos\,\alpha_s = 1.0$ if L_I represents a flow line orthogonal with the φ - isoline.

To exclude the impact of the direction in which curved L_I is digitized ($s = 1,2,\ldots N_s$ or $s = N_s , N_{s-1} ,\ldots 1$), the mean values of $\sin\,\alpha_s$ and $\cos\,\alpha_s$ are used:

$$\sin\,\alpha_s = 0.5\,(\,|\sin\,\alpha_{s,s+1}| + |\sin\,\alpha_{s-1,s}|\,)\,, \qquad \cos\,\alpha_s = 0.5\,(\,|\cos\,\alpha_{s,s+1}| + |\sin\,\alpha_{s-1,s}|\,. \tag{11}$$

The formulas of $\sin\,\alpha_{s,s+1}$, $\cos\,\alpha_{s,s+1}$ are the ones of (10). In these formulas for $\sin\,\alpha_{s-1,s}$ and $\cos\,\alpha_{s,s-1}$, the indices $(s + 1) \rightarrow (s - 1)$ should be switched. The absolute values of the trigonometric functions are used, in order to deal with $0.5\pi \geq \alpha \geq 0$ only. In the general case, the above formulations for (9), (10) cannot provide the right signs for i_{sn} , i_{st}. To detect possible mistakes the other version of (9) is provided where absolute values of i_{sn} , i_{st} are used.

5 COMPUTING FLOWS THROUGH AQUITARDS

The summary flow I_S^z through an aquitard area S_L framed by a closed line L is provided by the following formula:

$$I_S^z = \sum_{j=1}^{N_L} i_j\,, \qquad\qquad i_j = a_{zj}\,(\varphi_{z-1} - \varphi_z)_j\,, \tag{12}$$

where $j = 1, 2, \ldots, N_L$ are the numbers of the grid nodes belonging to S_L ; a_{zj} - is the element of A_z at the j-th node; $(\varphi_{z-1} - \varphi_z)_j$ is the computed head difference on the aquitard here.

To detect the nodes belonging to S_L , the special mask is applied. It is provided by the GDI program (Spalvins & Slangens 1995).

6 CONCLUSION

For the REMO system, four new subsidiary software tools have been developed. All of then are based on a line as an information carrier. The tools enable to improve the HM formulation and flow balance calculations. The tools have been successfully applied in the course of practical projects.

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Spalviņš A., Šlangens J., Janbickis R., Lace I. Jaunas palīgprogrammas modelējošajai sistēmai REMO.
Modelējošajā sistēmā REMO iekļautas jaunas palīgprogrammas. Tās var izmantot hidroģeoloģisko modeļu formulēšanai un pazemes ūdens plūsmu balansa aprēķiniem.

Спалвиньш А., Янбицкий Р., Шланген Я., Лаце И. Новые вспомогательные средства для моделирующей системы REMO.
Для моделирующей системы REMO разработаны новые вспомогательные программы. Они могут быть использованы для формулировки гидрогеологических моделей и расчетов баланса потоков подземных вод.