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title: **Creating of regional hydrogeological model for the south-east of Lithuania**

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INTRODUCTION

To fulfil the European Commission water directives (98/83EC, 2000/60EC), Lithuania has prepared the program (2007–2025) focused on improving management of its rich groundwater resources and on supplying the country with drinking water of high quality. The program includes the task to evaluate groundwater resources by processing accumulated hydrogeological data by methods of mathematical modelling. For the first time, the regional hydrogeological model (HM) has been developed for the Quaternary groundwater system located in the South-East of Lithuania (Figure1). This groundwater body covers one third of the country. The rectangular HM area has the size 290km×210km= 60900 km^2. Local river basins comprise the active HM area of highly irregular shape (Figure2). The model area, exterior to the active one, does not take part in simulation.

Figure 1. Model location.

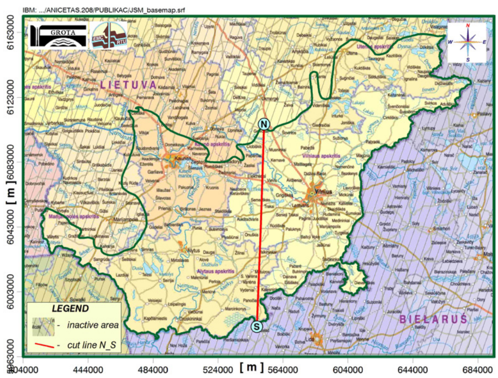

Figure 2. Model area (290km×210km, h=0.5km).

The Quaternary groundwater system to be modelled is highly irregular (Figure 3). To account for its complexity, HM contains 11 layers (planes). The finite difference 3D scheme is applied with the plane approximation step h=500 metres. Therefore, the HM grid plane contains 481×421=244601 nodes and the HM 3D grid includes 2690611 nodes. The Groundwater Vistas (GV) system (Environmental Simulations Inc., 2007) was used for creating of steady state HM that simulated the mean annual hydrogeological conditions.

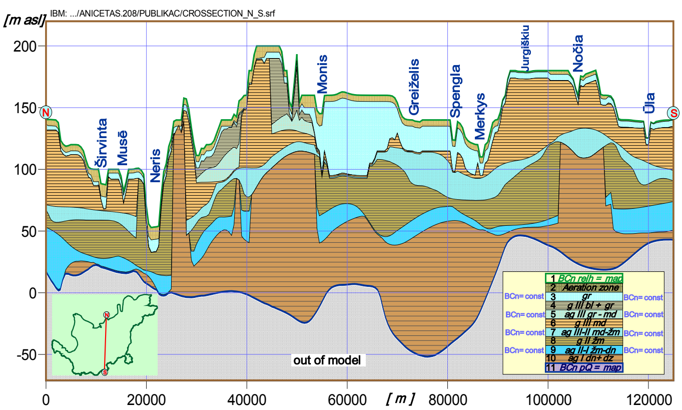

Figure 3. Geological cross section NS.

To create HM, two new methods were applied: 1) by using the ground surface elevation map, as the boundary condition, the feasible infiltration distribution was obtained; 2) in the "start on" version of HM, the uniform flat layers were applied to substitute the real geometry of HM. The real geometry can be accounted for later, by using grid calculations which transform permeability maps of calibrated HM containing flat layers. This extended thesis is based on information given in the publication (Spalvins et al., 2009).

BASIC MATHEMATICS OF HM

To consider the process of the HM creating, its basic matrix mathematics is presented by the following algebraic equation system:

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

where φ is the solution vector (heads) at nodes of HM grid; A – the symmetric sparse matrix of the geological environment presented by the xy-layer system containing horizontal (A_{xy} - transmissivity) and vertical (A_z – vertical hydraulic conductivity) elements of the grid; ψ - the boundary head vector, which includes ψ_{top}, ψ_{bot} and ψ_{bound} - subvectors on the HM top, bottom and borderlines, accordingly; G – the diagonal matrix (part of A) which elements links the nodes where φ must be found with the ones where ψ is given; β - the boundary flow vector.

By using the 3D finite difference approximation, the xyz grid of HM is built using ($h\times h\times m$) - sized blocks (h is the block plane size; m is the variable thickness of a layer).

The elements a_{xy}, a_z of A_{xy} A_z (or g_{xy}, g_z of G) are computed by using the following formulas:

$$a_{xy}=km, \qquad a_{zy}=(h^2k)/m, \qquad m_i=z_{i-1}-z_i>0, \qquad i=1,2, \quad s, \tag{2}$$

where z_{i-1}, z_i are the elevations of the top and bottom surfaces of the i-th geological layer; z_0 represents the ground surface elevation map $\psi_{top} = \psi_{rel}$ with the hydrographical network included; k, m are, accordingly, elements of digital m, k-maps of the computed layer thickness and permeability; s – the number of layers.

The set of z-maps describes full geometry of HM. It is built incrementally: $z_0 \rightarrow z_1 \rightarrow \ldots \rightarrow z_s$ by keeping the thickness of the i-th layer $m_i>0$. If in some areas $m_i=0$, then the i-th layer is discontinuous. To prevent "division by zero", in the a_z calculation of (2), $m_i=0$ must be replaced by $\varepsilon>0$ (for example, ε = 0.02 metres). In GV, only the z-maps serve as the geometrical ones (no m-maps accepted).

Two tasks of the HM creating are the most difficult ones: obtaining the distribution for the infiltration flow β_{inf} on the HM top; building the z-map set.

For reported HM, these tasks were considerably eased, as follows:

- by using the ψ_{rel} –map, a feasible infiltration flow was obtained, as a part of the solved system (1);
- no real z-maps were applied, until the HM calibration was finished.

When ψ_{rel} is used, the flow $\beta_{aer} = \beta_{inf}$ passes through the aeration zone:

$$\beta_{aer} = G_{aer}(\psi_{rel} - \varphi_Q) \tag{3}$$

where φ_Q is the computed head (subvector of φ) for the first Q aquifer; G_{aer} submatrix of G contains the vertical ties g_{aer} of the aeration zone connecting ψ_{rel} with φ_Q. The expression (3) reflects the response of HM, if the ψ-condition is applied. As a rule, even the first run of HM provides good results for β_{aer} that can be easy calibrated.

For calibrated HM, its real geometry can be accounted for by applying the following grid data transformation for k_{xy}, k_z-maps:

$$k_{zy}=(km_c)/m, \qquad k_z=(k_z/m)_c m \tag{4}$$

where $(km)_c$, $(k_z/m)_c$ - the calibrated transmissivity and vertical leakance values, accordingly; m – the real thickness of a layer. The transformation (4) does not change flows and heads of calibrated HM.

DESCRIPTION OF HM

Boundary conditions of the ψ -type were applied on the top and bottom HM planes (1st and 11th), on the borderline of the active HM area (planes 3, 5, 7, 9 of aquifers). The ψ_{rel}-map carried by the plane 1 regulates the infiltration flow which distribution is highly irregular. The plane 2 represents the aeration zone as a formal aquitard with a variable permeability. Its distribution was obtained during HM calibration. The plane 3 simulates the first unconfined Quaternary aquifer. The next three aquifers (planes 5, 7, 9) are the confined ones. The planes 4, 6, 8, 10 simulate aquitards that control vertical groundwater flows passing between aquifers. The hydrographical network was implemented in the plane 3 and in the plane 1 as a part of the ψ_{rel}-map. The HM bottom plane 11 carries the ψ_{pQ} -map that represents the pre-Quaternary piezometric heads.

To run the GV program, it is necessary to feed into it the following maps and data files: the surface elevation digital maps of layers (z-maps), the permeability maps (k-maps), the boundary conditions for the planes 1 and 11 (ψ-maps), the ψ_{bound} data for the active area borderline (planes 3, 5, 7, 9), the groundwater withdrawal data β_w for well fields.

To gain time for building the z-maps, and not to postpone creating of HM, the uniform flat layer system was used instead of the real one. Because all layers of this simplified HM version have the thickness m_c=1.0, the transmissivity km-maps were used instead of the k-maps for creating elements of the matrix A_{xy}. For aquifers, the km-maps of good quality were available. For aquitards, the A_{xy} elements were insignificant, because of their small permeability values ($10^{-2}>k_0>10^{-5}$) m/day.

Unfortunately, no data were available of the aquitard permeability k_z for A_z elements. As the first try, the k_z-maps were used where $k_z=k/m$ (m – an expected thickness of a layer). In areas where m=0, large values $k_z=10^5$ m/day were applied, to connect tightly the neighboring layers.

CALIBRATION OF HM

Finding and correcting errors occurring in the ψ and β-maps of boundary conditions were the first tasks to be done, because no calibration could eliminate this type of faults. Searching for the right k_z-maps of aquitards were the main object of HM calibration.

Two kinds of calibration targets were applied: the observed heads; the mean subsurface runoff rate of river basins. In Tables 1 and 2, the calibration results for both groups of targets are presented. As the calibration targets for heads, 823 monitoring wells were used. Satisfactory match was achieved between observed and modeled heads. The standard deviation was within the range (2.49-3.08) metres; the relative deviation obtained as "standard deviation/observed range" did not exceed 1.8%.

Table 1. Target statistics for calibrated heads.

Nr. of layer	Number of targets	Residual mean [m]	Standard deviation [m]	Observed range in heads [m]	Relative deviation [%]
3	357	-0.11	2.53	210.2	1.2
5	104	-0.41	3.08	190.5	1.6
7	189	-0.19	2.91	192.5	1.5
9	173	-0.46	2.49	138.8	1.8
Total	**823**				

Not all available head targets were used, because of the following reasons:

- hence the HM grid was not detailed enough (h=500 m), in areas where the φ-distribution was steep, it could not reproduce the monitored heads correctly;
- in the vicinity of well fields, the head observations of previous years could not reproduce the modeled ones, because nowadays the water withdrawal rates had dropped considerably;
- considerable influence of the seasonal head changes, especially, for the first aquifer (plane 3).

Table 2. Subsurface runoff rate for river basins.

River basin	Area of river basin in model [km^2]	Expected subsurface runoff rate [l/s km^2]	Modelled subsurface runoff rate [l/s km^2]	Relative error [%]
Neris	3529	3.80	4.03	6.0
Merkys	2860	5.16	5.18	0.6
Zeimena	2693	4.45	4.39	1.4
Nemunas	6054	3.37	3.30	1.9
Sesupe	1676	1.34	1.41	4.7
Sventoji	1186	2.82	2.46	13.5

It follows from Table 2 that HM satisfactory reproduces the mean subsurface runoff rates for the six river basins. The maximal relative errors 31.6% and 13.5% are for the Neris and Sventoji basins, respectively.

CONCLUSIONS

The regional hydrogeological model has been built for the South-East of Lithuania. It simulates the Quaternary groundwater body that represents the main source of drinking water for this part of country.

The model was created by applying an innovative methodology that enabled to shorten the time for building of this complex model.

The model is open for possible improvements and it also serves as a base for creating local models of well fields, and for the areas where sanitation measures of contaminated places should be evaluated.

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