# METHODS AND TOOLS TO BE APPLIED FOR CREATING OF REGIONAL HYDROGEOLOGICAL MODEL OF LATVIA

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**ABSTRACT**

The hydrogeological model of Latvia will be established during 2010-2012. It will be used for management of drinking groundwater resources in order to implement standards of European Union Water Directives. The model will be created in environment of the commercial program Groundwater Vistas. It includes the broadly used software tools. The area to be modeled is represented by $951 \times 601 \times 25$ finite difference grid, which plane approximation step is 500 metres. Novel methods and software tools will be applied to create the highly complicated model: the map of the ground surface elevations will serve as the piezometric boundary condition for obtaining distribution of infiltration; for creating digital maps of the model initial data, original software tools of data interpolation will be used; in the initial phase of the model establishment the actual geometry of a model may not be applied.

**INTRODUCTION**

The countries of the world and of the European Union are developing hydrogeological models (HM) where, by means of computer modeling, the information necessary for the groundwater management planning is obtained (Motz and Gan. 2002, Farell et al. 2007, Snepvangers et al. 2007, Spalvins et al. 2010).

Even though Latvia is rich in surface water as well as in groundwater, the planning of the state water resources management is obligatory, in order to match the aims of the European Union Water Directives. HM of Latvia will be established as the element of the Latvian shared environmental information system. The model will be used for the regional drinkable groundwater resources management and for evaluation of their recovery measures. To solve problems of a smaller scale, regional HM will serve as the data source for building more detailed local models.

The model will be established by the team of the Environment modeling centre (EMC) of the Riga Technical university. The EMC team has taken part in creating HM of regional scale in Latvia and abroad: HM REMO for the central part of Latvia (Spalvins et al. 1996); HM of the Noginsk district, Russia (Spalvins et al. 2001); HM of the south-east of Lithuania (Spalvins et al. 2010). In Figure 1, locations of Latvia HM and of REMO are shown.
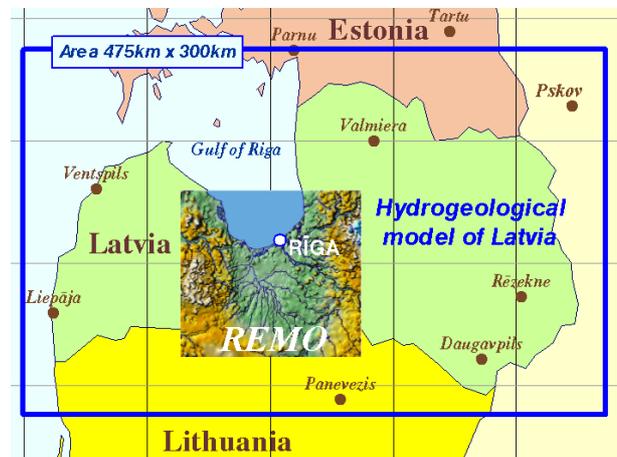


Figure 1: Location of Latvia HM and REMO

An innovative methodology and software tools allowing reducing uncertainty of results given by HM and simplifying the model calibration process will be applied.

If the traditional methodology is used, the first groundwater horizon on HM needs a map of atmospheric infiltration distribution and digital maps of surfaces for all geological layers must be obtained (a very complicated task in the case of Latvia). Unfortunately, modelers never have reliable data for the regional infiltration distribution. That is why this map is obtained as a product of an exhausting calibration process. However, usually then results of HM have a significant uncertainty.

If, as a piezometric boundary condition, a map of ground surface relief with incorporated elements of a hydrographical network is used, the model itself forms a highly reliable infiltration map that can be corrected by changing filtration characteristics of the aeration zone (Spalvins et al. 2001). For the Lithuania project (Spalvins et al. 2010), a method was successfully used that does not require geological layer surface maps (at

least, at the beginning of the model construction). A novel method will be applied, to account for the fact that effective thickness of a layer may be smaller than its geometrical thickness, due to presence of isotropic inclusions, (Spalvins et al. 2009). Original software tools developed by the EMC team will be applied for obtaining digital maps of HM initial data (Spalvins et al. 2004). To ensure compatibility with models of other countries, the commerceial program "Groundwater Vistas" (GV), is used for establishing of HM (Environmental Simulations, 2007). The GV program is regularly updated. It includes a broad range of specialized software (MODFLOW, MODPATH, MT3D, etc.) used throughout Europe and globally.

HM of Latvia covers the 475km×300km area. HM contains 25 approximated geological layers (including the relief as an aquifer). The 3D finite difference approximation is used. Its plane step h=500 metres. Therefore, the HM grid contains 951×601×25=14288775 nodes.

If the quasi 3D approximation is used (as in HM REMO) then the number of HM planes can be reduced from 25 to 13. There twelve planes of aquitards are replaced by vertical links. However, such HM cannot rightly co-operate with the MODPATH and MT3D software accounting for transportation processes.

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## BASIC MATHEMATICS OF HM AND NEW METHODS

To describe creating of HM, the mathematics of the 3D-steady state model must be introduced. By applying 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 geological layer). The model constitutes a rectangular $p$-tiered xy-layer system where $p$ is the number of layers. Four vertical sides compose the shell of the HM grid. The relief (ground surface) and the lower side of the model are its geometrical top and bottom, respectively. The 3D-space volume enveloped by the boundary surfaces constitutes the body of HM.

The vector $\varphi$ of the piezometric head is the numerical solution of the boundary field problem which is approximated in nodes of the HM grid by the following algebraic expression:

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

where $A$ is the symmetric sparse matrix of the geological environment which is presented by the xy-layer system containing horizontal ($A_{xy}$ - transmissivity) and vertical ($A_z$ – vertical hydraulic conductivity) elements of the HM grid; $\psi$ - the boundary head vector: $\psi_{rel}$, $\psi_{bot}$, $\psi_{sh}$ - subvectors on the HM top, bottom and shell, accordingly; $G$ – the diagonal matrix (part of $A$) assembled by elements, linking the nodes

where $\varphi$ must be found with the ones were $\psi$ is given; $\beta$ - the boundary flow vector.

The elements $a_{xy}$, $a_z$ of $A_{xy}$, $A_z$ (or $g_{xy}$, $g_z$ of $G$) are computed, as follows:

$$a_{xy} = k \times m, \quad a_z = \frac{h^2 \times k}{m}$$
$$m_i = z_{i-1} - z_i > 0, \quad i = 1, 2, ..., p \qquad (2)$$

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

The set of z-maps describes the full geometry of HM. It is built incrementally: $z_0 \rightarrow z_1, ..., z_p$ 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 the "division by zero", in the $a_z$ calculation of (2), $m_i = 0$ must replaced by $\varepsilon > 0$ (for HM, $\varepsilon = 0.02$ metres). In GV, only the z-maps serve as the initial geometrical ones.

Obtaining the right distribution for the infiltration flow $\beta_{inf}$ on the HM top is a burdensome task. For reported HM, this task is considerably eased by using the $\psi_{rel}$-map as the boundary condition for heads. Then the flow $\beta_{inf} = \beta_{aer}$ passes through the aeration zone:

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

where $\varphi_Q$ is the computed head (subvector of $\varphi$) for the first aquifer $Q$; $G_{aer}$ (diagonal submatrix of $G$) contains the vertical ties $g_{aer}$ of the aeration zone connecting $\psi_{rel}$ with $\varphi_Q$. The expression (3) gives the usual result of HM, when a $\psi$-condition is applied. As a rule, even the first run of HM provides feasible results for $\beta_{inf}$.

The elements $g_{aer}$ of $G_{aer}$ are computed, as follows:

$$g_{aer} = \frac{h^2 \times k_{aer}}{m_{aer}}, \quad m_{aer} = \psi_{rel} - \varphi_Q \quad if \ \beta_{aer} > 0$$

$$m_{aer} = 1.0 \quad if \ \beta_{aer} \leq 0 \qquad (4)$$

where $k_{aer}$, $m_{aer}$ are, respectively, the permeability and thickness of the aeration zone. Initially, $k_{aer}$, $m_{aer}$ are unknown. As the first try, the following values of these parameters may be applied: $m_{aer} = 1.0$ metre; $k_{aer} = 10^{-3}$ [m/day]. The lines and areas of the hydrographical network are implemented, accordingly, as rivers and lakes of the GV system. Their bed conductances (links with the HM grid nodes) must be calibrated. Formerly, the bed conductances were elements of the aeration zone. The innovation was implemented just recently (Spalvins et al. 2010).

To avoid iterative changes of the HM geometry, $m_{aer} = 1.0$ may be kept constant, until the calibrated state of HM is achieved. Only then, the real $m_{aer}$ must be

introduced. The $k_{aer}$-distribution is the object of HM calibration.

For geological layers, their geometrical thickness is $m \geq m_{ef}$. The effective thickness $m_{ef}$ accounts for the fact that, not always, the layer permeability is isotropic. Aquifers and aquitards may include admixtures, accordingly, of low and high permeability. Because the HM geometry is created on the thickness m-maps, the original $k_{xy}$, $k_z$-maps must be corrected, as follows:

$$(k_{xy})_c = k_{xy} \times C, \quad (k_z)_c = k_z \times C^{-1},$$
$$c_i = \left(m_{ef} \times m^{-1}\right)_i \leq 1.0 \tag{5}$$

where $(k_{xy})_c$, $(k_z)_c$ are the corrected permeability values; $C$ is the diagonal correction matrix which is obtained by interpolating borehole data on the xy-grid planes of HM; $c_i$ – the i-th initial element of $C$ given by a borehole. The algorithm of (5) has been firstly used to create HM of a new well field (Spalvins et al. 2009).

If no transport processes (migration of contaminants, particle tracking, etc.) are tried on HM, it is not necessary to apply its real geometry (Environmental Simulations 2007). If $m_c=1$ is fixed for all layers of HM, then instead of the original k-maps requested by formulas (2), the corrected ones of $k_c$ must be used:

$$k_c = m\, k = a_{xy}, \quad \text{for aquifers}$$
$$k_c = k / m \quad \text{for aquitards} \tag{6}$$

where $m$ and $k$ represent elements of the original m, k–maps. The transformation (6) does not change values of $a_{xy}$ and $a_z$ provided by formulas (2).

The above method was used by the EMC team, to start HM for Lithuania (Spalvins et al. 2010), because the z–maps were not ready from the very beginning of the project. However, rather good km-maps (transmissivity $a_{xy}$ of (2) were available for aquifers. Locations of the $m=0$ areas (windows) of aquitards were known. Both facts enabled to start calibration of HM by using the equal thicknesses $m_c=1.0$ for all HM layers. When the right z–maps were available, the HM calibration was already completed. Because it was necessary to introduce the real geometry of HM, the following "inverse" transformation for k–maps was used:

$$k_{xy} = (km)_c / m, \quad k_z = (k_z)_c\, m \tag{7}$$

where $(km)_c$ and $(k_z)_c$ were calibrated values of the $k_c$–maps. The above method, enabling to apply very simple HM geometry, will also be used for starting HM of Latvia.


## INTERPOLATION OF DATA

For the z, k – maps, interpolation surfaces represent geometrical images. Initially, for creating these maps, the EMC team managed to apply the wide known interpolation methods: Criging, Minimal Curvature, Inverse Distance. Unluckily, these methods sometimes provided evidently wrong results (Spalvins and Slangens 1994). For example, if an m-distribution was highly irregular, negative thicknesses appeared, even if the initial ones were strictly positive. It was understood that this unexpended failure was due to the following principal hindrances of these methods:

- interpolated results did not hold the maximum / minimum principle towards initial data applied;
- initial data were often overruled by practically uncontrollable algorithms applied for smoothing of the interpolation result.

Because conventional methods cannot provide strictly controllable interpolation results, the GDI program has been developed (Spalvins and Slangens 1994, Spalvins et al. 2007, Spalvins and Slangens 2007). It provides the interpolation surface σ, as the numerical solution of the following associated 2D − boundary problem, on the i−th plane of system (1):

$$div(\lambda\ grad\ \sigma)=0, \tag{8}$$

$$V\ \sigma = -G_\sigma\ \sigma_\psi, \qquad V=V_{xy} - G_\sigma \tag{9}$$

where (9) is the algebraic equation system, applied to approximate the problem (8); the matrices $V_{xy}$, $G_\sigma$ represent, correspondingly, the horizontal links $V_{xy}$ of the interpolation grid and the elements $g_\sigma$ connecting nodes where σ must be found with the ones where $\sigma_\psi$ are known. The parametre $\lambda(x,y)$ is used for controlling the shape of $\sigma(x,y)$. Due to the changeable $\lambda(x,y)$, it is possible to modify the « strength » for each initial data source $\sigma_\psi$.

The GDI program mostly applies various line data as the initial ones, because they are much more informative than few pointwise data the lines are based on. For example, information carried by the long line profile of a river is far richer than the measured water levels of the river applied for obtaining the profile.

In GDI, any line can also be used, as an impervious border that dissects the xy−area, if necessary (masking of polygons, etc.).

An original program CRP has been developed (see the next section) for preparing the line data (isolines, geological borderlines, data of hydrographical network and converting them into the initial data $\sigma_\psi$ of the GDI program (Slangens and Spalvins 2000).

The GDI program is mainly applied in the sequential mode. During the current interpolation step, new information is used, but the results of the previous step serve, as the base. In this way, much simpler set of initial data can be applied than if one tries to obtain the final result at once. To create very complex maps, even small sets of initial root data are sufficient.

Unlike most of interpolation methods, the surface created by GDI may include sharp edges that very often are a part of the z–maps (tectonic faults, etc.).

## PREPARING LINE DATA FOR THE GDI PROGRAM

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

$$L = \left\{ c_j \right\}, \qquad j=1,2, ...,J;$$

$$l_{I,J} = \sum_{j=1}^{J-1} l_{j,j+1},$$

$$l_{j,j+1} = \sqrt{(x_j - x_{j+1})^2 + (y_j + y_{j+1})^2} \qquad (10)$$

and $\{ c_j \} = \{ x_j, y_j \}$ is the coordinate set on the continuous $xy$-plane, of the master points where $L$ turns; $l_{I,J}$ and $l_{j,j+1}$ are the lengths, accordingly, of $L$ and the elementary vector linking the adjacent points $j$ and $j + 1$. The physical nature of $\sigma$ may be different (elevation $z$ of some surface, thickness $m$, or permeability $k$ of a geological stratum, etc.). The simplest graph of $\sigma$ is a horizontal line representing an isoline. Generally, the shape of $\sigma$ may be complex, such as elevation profiles of an eroded ground surface. If the additional points $t=1, 2, ...,T$ are introduced to approximate some curvilinear graph of $\sigma$ then the data line $L_\sigma$ including $J+T$ points (located on $L$), and $L_\sigma$ is specified, as follows:

$$L_\sigma = \{c_i, \sigma_i\}, i=1,2,...,J+T, \{c_i=c_j \wedge c_k\}, \{\sigma_i=\sigma_j \wedge \sigma_k\}. (11)$$

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

A special CRP program has been developed (Slangens and Spalvins 2000), due to the following reasons:

- in practice, rarely any line $L_\sigma$ is available in the arranged form of (11); some data processing is necessary to obtain this form;
- special calculations must be performed, to extract from (11) the particular duo set $\{c_s, \sigma_s\}$ where $c_s$ and $\sigma_s$ are the $xy$-coordinates and the $\sigma$-values, accordingly, at the intersections of $L_\sigma$ with the HM grid; this set represents the "$c$–data" applied by the GDI program for incorporating the lines into HM; the set $\{c_s, \sigma_s\}$ carries the line $L_s$, which approximates $L_\sigma$; proximity of these lines depends on the grid size, $h$ (finer grid $\rightarrow$ closer $L_s$ and $L_\sigma$).

The CRP program serves as a–preprocessor that prepares raw line data of (10) to the ones used by the GDI program.

The quality of the GDI-produced $z$-maps can be considerably improved if sections are applied massively, as reliable sources for the HM geometry. The special cross-section (CRS) program was developed in order to liberate the modeller from the routine task of preparing the sections for the GDI program (Lace and Spalvins 2000).

The section is composed of $p+1$ geological elevation $z$-profiles $L_z$, as crossings of the $z_i$-surfaces of (2) with the vertical plane of the section. In the $xy$-plane, the section is specified by its carrier - the broken line $L$ of (10) passing through the master wells.

An elevation profile $L_z$ is rarely drawn like a simple broken graph (in the vertical plane) where the master wells of $L$ are connected by straight lines. Usually, these connections are curved, due to some supplemental information added by a hydrogeologist, and the representation of (11) should be applied.

The set $\{ c_i, z_i \}$ of (11) must account for the following main characteristic points of the $z$-profiles:

- master wells $j$ of $L$;
- additional points for approximation of curvilinear $z$-profiles;
- cross-points with elements of the hydrographical network;
- cross-points with other sections applied;
- location of geological boundaries for discontinuous layers.

In practice, because of different reasons not considered there, no real section initially matches exactly the various data lines and points listed above. Errors are to be detected and corrected, possible minor discrepancies eliminated and initial data harmonized before they are run by the GDI program. This task is accomplished with the help of the CRS program, which is used, as the pre-processor of the CRP program. The main features of CRS are: making necessary alterations of the section, and preparation of the duo set $\{ c_i, z_i \}$ for $L_z$ by using its electronic image.

To alter the section, the coordinates $\{ c_j \}$ of (10) can be corrected and the length for each $l_{i,i+1}$ of (11) can be modified by introducing its scale factor $s_i$, as follows:

$$L\{ c_j \} \rightarrow L\{ ( c_j )_c \},$$

$$s_{I,N} l_{I,N} = \sum_{i=1}^{N-1} s_i l_{i,i+1} = \sum_{i=1}^{N-1} (l_{i,i+1})_c \qquad (12)$$

where $( c_j )_c$ and $( l_{i,i+1} )_c$ are altered coordinates of the master wells $j$ and the corrected lengths of elementary vectors of $L_z$, correspondingly; $s_{I,N}$ is the correcting scale factor for the full length of $L_z$. However, for the sake of simplicity, the original notations of (11) will be used in the further explanations, instead of the corrected ones of (12).

A digitizer program provides the duo set $\{ l_{1, i}, z_i \}$ containing the lengths $l_{1,i}$ and the $z_i$-values, at the current points $i$ of $L_z$. The CRS program founds the coordinates $c_i$, as follows:

- from the representation (10), the fragment $l_{j, j+1}$ is found where the point $i$ is located;
- the coordinates $x_i$ and $y_i$ are computed:

$$x_i = x_j + \delta_{j, i}(x_{j+1} - x_j), \qquad y_j = y_j + \delta_{j, i}(y_{j+1} - y_j),$$
$$\delta_{j, i} = l_{j, i}/l_{j, j+1}, \qquad 1 \geq \delta_{j, i} \geq 0, \qquad (13)$$

where co linearity of $l_{j, i}$ and $l_{j, j+1}$ (as vectors) are utilized. To simplify the CRS program control, all profiles of the section apply the common set of wells and additional points. The CRP program will be applied to create the z–maps for HM of Latvia.

## DIGITAL RELIEF MAP

Obtaining of the digital relief map $\psi_{rel}$ of Latvia (scale 1:200000) is a rather difficult task, because the maps prepared by the Geospatial Information Agency of Latvia still do not account for existence of the hydrographical network. Three versions of the maps are available: a) and b) are digital elevation maps (DEM) with regular grid cell sizes 20m and 70m, accordingly; c) vectored 1:50000 scale topographical maps where surface elevation data are presented by isolines (IEM).
By using the b-DEM and IEM versions, the EMC team is going to obtain the digital $\psi_{rel}$–map, as follows:

- from b-DEM, the "terrestrial" DEM version is found, on the HM xy–plane (cell size 500m);
- elements of the hydrographical network are constructed;
- by using the GDI program, the hydrographical network is incorporated into terrestrial DEM.

Unfortunately, no usable data needed for obtaining the hydrographical network are available and they must be extracted from the b-DEM and IEM versions:

- the set of rivers and lakes, to be included in HM, must be formed;
- by manual digitizing, middle line coordinates of rivers must be obtained from b-DEM where rivers are presented by chains of polygons; this kind of river record is not acceptable for the GV system; codes of shorelines of lakes can be taken directly from b-DEM;
- by finding crosspoints of the river middle lines with isolines of IEM and by applying the algorithm described in (Slangens et al. 2010), initial data can be found for constructing the long profiles of rivers by the CRP program; lakes included in HM are rather large and their levels are known. However the algorithm mentioned above, also can find unknown levels of small lakes.

The elements of hydrographical network are applied as line and area data carriers that complement the terrestrial DEM version of HM.

## CALIBRATION OF HM

Due to unavoidable limitations in the initial data, HM has no unique solution. Calibration of HM is a controlled iterative process involving the addition of complimentary data, until as HM of a required quality is obtained. The quality is checked and maintained by tracing calibration targets. The following targets are usually applied:

- original data should not be contradicted by data generated by HM; for example, the $\psi$ and $\varphi$ distributions of (1) must reproduce observed head values, the matrix A must incorporate observed permeability and geometrical features of k, z–maps, etc.;
- within the HM body, groundwater flows should not reach unnaturally large values (infiltration flow, flows regarding the hydrological network, etc.);
- results of HM must confirm the real hydrogeological situation, because formal agreement between computed and observed target data does not assure correct simulation; unfortunately, automatic calibration tools can sometimes provide almost worthless results.

The first and second targets are formal components of HM, but the third target always requires subjective evaluation.
The calibration will never succeed if serious HM errors are present. Problems can include faults in data coordinate or values, mistakes in the identify of geological layers, mismatched reference data, unreliable boundary conditions or inadequate software.
Where initial data have not been previously used for modeling (most of data, to be used for HM of Latvia, belong to this group), their role can be unclear and their validity may be questionable (especially, the stratigraphical data of boreholes).
However, to create and calibrate HM, the EMC team is going to apply already tested sophisticated methods and software tools, in order to overcome possible problems regarding quality of initial data.

## CONCLUSIONS

During two years (till 2012) the EMC team of the Riga Technical university, Latvia should establish the regional hydrogeological model of Latvia. The model will be applied as the element of the shared environmental information system. To create the model the EMC team is going to use innovative methodology and software tools. The following main innovations will be used:

- the improved method of creating infiltration flow;
- the method for accounting for the effective thicknesses of geological layers;

- the method that enables not to use the real geometry of HM (at least, in the beginning);
- improved original software tools for interpolation of geological and geometrical data;
- the method enabling to found data needed to create the hydrological network of HM.

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