Know – how technologies developed for modelling hydrogeological processes

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ABSTRACT: Since 1993, the team of the Environment Modelling Centre (EMC) of the Riga Technical University has been active in developing special software for creating hydrogeological models (HM). These new tools have been applied in conjunction with commercial ones for solving practical problems regarding drinking water supply and dynamics of contaminated groundwater. The new software tools and main projects EMC has dealt with are considered.

1 INTRODUCTION

For modelling hydrogeological problems, the EMC team has applied deterministic methods, and mainly steady state problems have been considered, because the EMC projects usually dealt with long-term processes. However, the software and methods developed by EMC may also be applied for modelling transient groundwater flows.

To describe results of EMC, some mathematics of semi-3D steady state HM is considered. The xyz-grid of HM is built of \((h \times h \times m)\)-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 of interjacent aquitards separating these aquifers. Its 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 a boundary field problem, describing the 3D-groundwater flow approximated in nodes of the HM grid, by the following algebraic equation system:

\[
A \varphi = b, \quad A = A_{xy} + A_z - G, \quad b = \beta - G \psi, \quad \beta = \beta_{in} + \beta_{bot} + \beta_{sh} + \beta_{w}, \quad \beta_{\psi} = G (\psi - \varphi)
\]

where the matrices \(A_{xy}, A_z, G\) represent, correspondingly, horizontal links \(a_{xy}\) of aquifers (arranged in \(xy\)-planes), vertical ties \(a_z\) originated by aquitards, elements \(g_{xy}, g_z\) connecting nodes of the grid with the piezometric boundary conditions \(\psi\) specified on some HM areas (\(\psi\)-surfaces); the vector \(\beta\) accounts for boundary flows: \(\beta_{w}\) is the water production rate in wells; \(\beta_{in}, \beta_{bot}\) and \(\beta_{sh}\) are the boundary flows, which may be specified on some areas (\(\beta\)-surfaces) of top, bottom, and shell surfaces, accordingly; \(\beta_{\psi}\) is the computed flow passing through the elements of \(g_{xy}, g_z\) forming the diagonal matrix \(G\).

Each grid plane contains \(n_{xy} = n_x \times n_y\) nodes \((n_x\) and \(n_y\) represent, accordingly, the number of nodes on \(x\) and \(y\) sides of the plane). Thus, the whole grid of (1) contains \(N = n_{xy} \times (s+1)\) nodes, because only the neighboring nodes are interconnected. The matrix \(A\) contains no more than \(7N \approx N^2\) nonzero elements (usually, \(N = 10^3 \div 10^6\)). The elements \(a_{xy}, a_z\) of symmetric \(A_{xy}, A_z\) (or \(g_{xy}, g_z\) of \(G\)) are computed, as follows:

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

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 \(\psi_{rel}\) with the hydrographical network included; \(m, k\) are, accordingly, elements of digital \(m, k\)-maps of the computed thickness and permeability of layers.
The set of the $z$-maps describes the full geometry of HM. It is built in the consecutive way: $z_0 \rightarrow z_1 \rightarrow \ldots \rightarrow z_{2s+1}$, by keeping the thickness of the $i$-th layer $m_i \geq 0$. If in some area $m_i = 0$ then this $i$-th layer is discontinuous. In modern modelling systems, the $m$-maps are never computed directly from data of geological thicknesses, because this approach may result in serious errors of the HM geometry.

All constituents of (1) are HM results. Creating and simulation of them can be conditionally parted into the following stages where some specific errors may occur:

- the pre-processing (model formulation) of (1); unfortunately, initial data provide information for a limited set of points and lines only, and to create HM, some HM calibration should be used;
- obtaining of $\phi$ by a special solver programme;
- post-processing of the HM results.

Faults of the model formulation are the dominant ones, and they are also interdependent with the errors of solving and post-processing. The methodology of subduing all types of HM errors has been considered in [15, 17, 18]. For this reason, this problem is not viewed in this paper.

Due to unavoidable incompleteness of initial data, the task of creating real HM has no unique solution. The number of formally rightful systems (1) is not limited. Calibration of HM is a controlled iterative process of adding complementary initial data enabling to obtain HM of a required quality. The quality is checked and maintained by tracing calibration targets. The following targets are mainly applied:

- original initial data should not be contradicted by the ones provided by HM; for example, the $\psi$ and $\phi$-distributions of (1) must reproduce observed head values; the matrix $A$ must incorporate observed permeability and geometrical features of (2), etc.
- results of HM must confirm the real hydrogeological situation, because no formal agreement between computed and few observed target data can assure actual correctness of simulation; unfortunately, automatic calibration programmes sometimes may provide practically worthless results;
- within the HM body, groundwater flows should not reach unnaturally large values;
- if HM serves, as a driver for a mass transport model then HM should be specially adjusted, to account for particulars of these transport processes.

The first and third targets are formal, but the second one always needs a human estimation, which is ever individual. Therefore, the accepted final HM results should be always subjective due to such a human assistance.

The calibration cannot be ever successful if serious HM errors are present (faults in data coordinates or values, mistakes in attachment to geological layers, mismatched data reference systems applied, unreliable boundary conditions or inapt software used, etc.).

Creating of HM forces a team of modellers to check up and systematize all initial data available. Moreover, important supplementary information is added via the calibration. Only then (especially, for 3D problems) HM becomes functional and can provide reasonable results. If some initial data have never been used for modelling, their rightfulness has not been tested within an interlinked system of data. This is a serious drawback of any unverified hydrogeological database, which may contain a lot of crude undetected errors.

Since 1993, the EMC team has been involved in various practical projects (Table 2). It was necessary to create numerous complex HM, and a rather rich set of new methods and software were developed (Table 1). The paper provides an insight both on the projects and the new tools.

2 GENERAL SCHEME. SUMMARY OF SOFTWARE APPLIED

The scheme applied by the EMC team for formulating of HM includes the following main stages and tools:

- scanning hard copies of necessary maps, in order to convert them into electronic images; digitizing the electronic images of maps; any digital map is based on a rather limited set of vectored line and point initial data which are sufficient for creating of the map at nodes of the HM grid;
- computing the geological $z$-surfaces of (2); if the HM geometry is complex, this is the most time-consuming part of the HM making [4, 13]; the Geological Data Interpolation (GDI) program [14] supports this part;
- construction of $k$-, $\beta$- and $\psi$-distribution maps; applying of these maps for HM calibration; the modelling system REMO [13] is applied at this stage, and all calibrated HM results become available for further utilization;
- the contaminant mass transport is modelled by the Groundwater Vistas (GV) and ARMOS systems [2, 29]; the HM data for them are taken from REMO.
- the SURFER program [3] is used for supporting graphics, digitizing of electronic images, and performing grid mathematics.

It was necessary to develop special tools, listed in Table 1, because the available commercial ones (for example, MODFLOW [9] and interpolation modules of SURFER) turned out to be insufficient for handling of practical cases involving complex hydrogeological systems [1]. Even today, many of the advanced modeling programs (like GV) are including some outdated principles inherited of the slow computer era: the zone scheme for saving memory [12]; the pure $\beta$-condition applied, as the infiltration flow $\beta_{in}$; on the HM top [11]; an unnecessarily strong human involvement required [17, 18], etc. This may cause serious trouble, when one tries to apply the GV system for creating HM, in a straightforward manner [4], without applying special novel tools.

In Table 1, the special tools are conditionally sorted into programs and methods. The method represents a serviceable algorithm, which can be utilized by any affixed program, even the commercial one. The column “Related software” gives the code of connected program - the user of the results provided by the program (or method) considered. For example, the REMO results may be exported to the GV program, or graphed by SURFER.

<table>
<thead>
<tr>
<th>Nr</th>
<th>Name of program or method; its function, [reference, section Nr]</th>
<th>Related software</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Program REMO; modelling and calibration of (1), [13, section 4]</td>
<td>GV, SURFER</td>
</tr>
<tr>
<td>2</td>
<td>Program GDI; creating interpolated data surfaces for (1), [14, section 5]</td>
<td>REMO, GV, SURFER</td>
</tr>
<tr>
<td>3</td>
<td>Program CRP; preparing line data and joining them with the HM grid, [10]</td>
<td>GDI</td>
</tr>
<tr>
<td>4</td>
<td>Program CRS; preparing line data of geological sections, [6]</td>
<td>CRP</td>
</tr>
<tr>
<td>5</td>
<td>Program INT$\beta\phi$; interpolates $\beta$ and $\phi$ values from irregularly located wells to nodes of the HM grid and backwards, [7]</td>
<td>REMO</td>
</tr>
<tr>
<td>6</td>
<td>Program INT$\beta$; interpolates $\beta$ values from irregularly located wells to nodes of the HM grid, [4]</td>
<td>GV</td>
</tr>
<tr>
<td>7</td>
<td>Program GVR; creates images of vertical cross sections of HM results along any line chosen, [13]</td>
<td>REMO</td>
</tr>
<tr>
<td>8</td>
<td>Program NFCG; solves the system (1), [5]</td>
<td>REMO</td>
</tr>
<tr>
<td>9</td>
<td>Method of using the ground surface elevation map, as the $\psi$-distribution, on the HM top, [11, section 6]</td>
<td>REMO, GV</td>
</tr>
<tr>
<td>10</td>
<td>Method of using the HM shell, as an interpolation device of the $\psi$-distribution, [16, section 7]</td>
<td>REMO, GV</td>
</tr>
<tr>
<td>11</td>
<td>Method of tuning zone converter modules, [12, section 8]</td>
<td>GV</td>
</tr>
</tbody>
</table>

It follows from Table 1, that all tools, but the Nr 6 and Nr 11 ones, provide data for, or support the REMO program, which is able to accomplish highly complex tasks (see section 4).

Due to resourceful methods of mathematical physics embodied, the GDI program can provide complicated interpolated surfaces (including the interlinked $z$-surfaces of discontinuous layers) by applying minimal sets of input data [15, 17] (see section 5).

The remarkable GDI-results are also due to the extensive use of various line data (isolines, geological boundaries and profiles of sections, long lines of rivers, etc) as the input for GDI. These data are computed by the CRP program, at intersections (cross-points) of lines (carriers) with the HM grid. The novel CRP version insures high quality of coordinates and values of data, at the cross-points.

The CRS program serves for editing data of vertical cross sections when they are applied as inputs for making of HM.

The INT$\beta\phi$ program considerably improves accuracy of REMO results, in the following way:
- boundary $\beta_w$-values of irregularly located wells are interpolated to four nearest nodes of the HM grid (GV roughly moves the $\beta_w$-value to the one nearest grid node!);
- in order to increase accuracy of the HM calibration, $\phi$-values can be computed at irregularly (with respect to the HM grid) sited observation wells; the GV code does not provide such a possibility.
The subsidiary INT\(\beta\) program considerably improves the \(\beta_w\)-distribution for the GV code by applying the REMO interpolated \(\beta\)–values, as the formal production wells, at nodes of HM.

It was necessary to develop the CRV program, because the GV system could provide sections for HM results only along the HM grid lines. Moreover, these GV produced sections may be quite erroneous [15].

Like the REMO solver, the NFCG program is a robust, reliable tool. From a modeller, no adjustments of its regimes are required.

The methods Nr 9 and Nr 10 present a breakthrough in modelling of hydrogeological processes. Due to them, reliability of HM results has raised drastically (see sections 6 and 7).

It was necessary to develop the method Nr 11, to avoid serious side effects caused by the zone memory scheme used in the GV system (see section 8).

It follows from Table 1 that a rather comprehensive arsenal of tools has been developed for producing HM. Some of them (Nr 1, 2, 9, 10, 11) are briefly considered later.

## 3 BRIEF HISTORY OF PRACTICAL PROJECTS

Table 2 represents the list of main practical projects performed by the EMC team.

<table>
<thead>
<tr>
<th>Nr</th>
<th>Name of project, country</th>
<th>Years</th>
<th>Companions</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Development of the regional hydrogeological model &quot;Large Riga&quot;, Latvia</td>
<td>1993-1996</td>
<td>SGSL(^1), GEUS(^2)</td>
<td>[1, 13, 21]</td>
</tr>
<tr>
<td>2</td>
<td>Modelling new well fields for water supply of Riga, Latvia</td>
<td>1996</td>
<td>SGSL, GEUS</td>
<td>[20, 22]</td>
</tr>
<tr>
<td>3</td>
<td>Modelling groundwater flow dynamics and contaminant transport for the Rumbula airbase place, Latvia - dynamics of free oil phase, its volume estimation - free oil recovery measures - mass transport of dissolved oil products</td>
<td>1996-2000</td>
<td>Hedeselskabet, Denmark, MEPRD(^3)</td>
<td>[23]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2000</td>
<td>VentEko, Latvia</td>
<td>[26]</td>
</tr>
<tr>
<td>4</td>
<td>Modelling of contaminant transport and remedy for the Ilukste oil terminal, Latvia</td>
<td>1997</td>
<td>Baltec Associates, Latvia</td>
<td>[23]</td>
</tr>
<tr>
<td>5</td>
<td>Development of contaminant transport models for sulphuric acid tar waste disposal sites in Incukalns, Latvia</td>
<td>1998</td>
<td>MEDRD, Baltec Associates, Latvia</td>
<td>[27]</td>
</tr>
<tr>
<td>6</td>
<td>Modelling of groundwater flow dynamics and contaminant processes at area of Vilnius oil storage, Lithuania</td>
<td>1998</td>
<td>GROTA, Lithuania</td>
<td>[28]</td>
</tr>
<tr>
<td>7</td>
<td>Hydrogeological and contaminant transport models for Noginsk district, Moscow region, Russia</td>
<td>1999</td>
<td>GEUS, VSEINGEKO(^4)</td>
<td>[4, 8]</td>
</tr>
<tr>
<td>8</td>
<td>Modelling of groundwater flow dynamics and contaminant transport processes for the Bernau area, Germany</td>
<td>2001</td>
<td>INGAAS GmbH, Germany</td>
<td></td>
</tr>
</tbody>
</table>

Abbreviations: 
1) SGSL - State Geological Survey of Latvia; 
2) GEUS - Geological Survey of Denmark and Greenland; 
3) MEPRD - Ministry of Environmental Protection and Regional Development of Latvia; 
4) VSEINGEKO - All Russian Research Institute of Hydrogeology and Engineering Geology

The first project (1993 -1996) was devoted to regional HM "Large Riga" created for investigating groundwater reserves and the existing water withdrawal interference of Latvia and Lithuania. This HM comprises 168 km \(\times\) 156 km = 26,208 km\(^2\) and includes the central part of Latvia, the northern side of Lithuania, and a large area of the Gulf of Riga. In the vertical direction, HM contains 9 aquifers. Due to dipping of geological layers, 6 aquifers and their adjoining aquitards are discontinuous. The HM vertical size is about 650
metres. The uniform plane step \( h = 4.0 \) km is applied, and the HM grid contains \( N = 43 \times 40 \times 9 = 15,480 \) nodes. Because of the utmost complexity of HM "Large Riga", available at this time commercial software (MODFLOW [9], interpolation modules of SURFER [3], etc.) failed to produce reasonable results [1], and it was necessary to develop new, more effective tools for HM making. During the first project, the basic versions of tools Nr 1, 2, 3, 5, 7, 8, 9, 10 of Table 1 have been developed. Since 1996, these tools have been updated repeatedly. The model "Large Riga" has also been improved \((h = 4.0 \) km \( \rightarrow 2.0 \) km\) and applied latter, as the regional base for the projects Nr 2 and Nr 5.

The second project confirms possibility of introducing new productive well fields for water supply of Riga from subsurface sources. More detailed submodels of these well fields were incorporated, within regional HM "Large Riga".

The both above projects were strongly supported by the Geological Survey of Denmark and Greenland. They were performed jointly by the EMC team and the State Geological Survey of Latvia.

The third project (1996-2000) dealt with contamination problems of the former Rumbula airbase, which was located on the bank of the Daugava river, near from the central part of Riga. The Rumbula area was rather heavily polluted with aviation fuel. The project contained all necessary stages of the contamination modelling: 1) creating of 2D HM for the polluted area, modelling of the oil body movement, estimation of the spilled immiscible oil volume; 2) modelling of free oil phase recovery measures; 3) making of 3D HM, as a driver for modelling the mass transport of dissolved oil products towards the Daugava river.

The REMO and ARMOS [29] systems, accordingly, were applied for creating both HM and for modelling dynamics and recovery of the free oil body. The GV program was used for modelling migration of dissolved oil products. This task was accomplished by the rather universal MT3D type transport code [30] included in GV.

One should notice that transportation processes of free immiscible and dissolved oil products differ strongly. For this reason, the highly specialized ARMOS code should be applied if the light immiscible oil movement is to be considered. Particle tracing methods used by the MT3D code cannot cope with such a task.

The fourth project (1997) represents a sophisticated use of the ARMOS code for investigating active leakage of diesel fuel under complex hydrogeologic conditions of the Ilukste oil terminal, Latvia. The simulation results were used for optimizing remediation measures of the terminal area and even helped to discover an origin of the long-lasting fuel leakage.

The fifth project (1998) represented a milestone for the EMC team, because the GV system was firstly used for investigating mass transport of dissolved hazardous contaminants from two pools at the Incukalns place, Latvia. Hence the hydrogeological conditions of the place was complex, a hierarchy of 3D HM was used and developed: HM "Large Riga" \((h = 2.0 \) km\) \( \rightarrow \) regional HM for the Incukalns place \((h = 100 \) m\) \( \rightarrow \) two local HM for the waste deposit pools \((h = 20 \) m\). The regional and local models are now permanently used for developing methods for remediation of this heavily polluted place.

The sixth project (1998) improved skills of applying the MT3D type code for modelling migration of dissolved oil products at the area of the Vilnius Oil Storage, Lithuania. The geometry of 3D HM was exceptionally complex, and the vertical geological cross sections were massively applied for the first time, as the HM input. Manual editing of these sections was difficult.

The seventh project (1999) represented the professionally most complex case the EMC team had ever dealt with. It was necessary to create 3D HM for the Noginsk District, Moscow region, Russia. Noginsk HM accounted for 13 geological layers, and seven of them were discontinuous. This feature made creating of HM extremely difficult. The geological cross sections were massively used and the special tool Nr 4 were developed to edit them. HM incorporated large number of water production wells. In order to improve their simulation accuracy, the program Nr 6 were developed, as the modification of the more powerful REMO subsidiary program Nr 5. It was also necessary to develop the method Nr 11 of tuning the GV system memory zone converter, in order to exclude damaging side effects occurring in the process of importing beforehand-prepared files, into the GV system. To ensure high reliability of any HM maps prepared by the GDI program, the tool Nr 3 was considerably improved. Therefore, the EMC team had spend a notable effort, to create Noginsk HM.

The current practical project (2001) is a challenge, because it deals with dense (heavier that water) contaminants at the Bernau area (located not far from Berlin), Germany. The hydrogeological conditions to be modelled are complex. Because the place of interest represents a buried Quaternary valley. The migration of dense contaminants is governed not only by the groundwater flow, but also by the top surfaces of aquitards where dense contaminants accumulate and glide down slopeward.
It follows from the above material that the EMC team has dealt with a lot of practical cases. This involvement has stimulated improvement and development of software tools.

4 THE MODELLING SYSTEM REMO

The system REMO represents the main tool, which is supported by a rich set of synchronized subsidiary programs. REMO is also compatible with the widely used MODFLOW software. However, REMO differs with MODFLOW in the following aspects:

- the REMO system automatically performs several routine operations, which require manual input if other software is used;
- no automatic change of any element of (1) is allowed by REMO (like blocking by MODFLOW of "dried" cells or modifying of some boundary conditions), because such changes may destroy HM if it simulates multilayered discontinuous geological structures;
- REMO does not apply the zone memory scheme;
- REMO applies the ground surface elevation map as a reliable piezometric boundary condition of the \( \psi \)-type;
- the REMO shell acts like an interpolation device; this feature is very helpful if HM contains discontinuous layers;
- calibration of \( A \) is performed mainly via the adequate iterative adjustment of \( k \)-maps, while the initial HM geometry is kept untouched, until the desired result is achieved; only then, if necessary, the real HM geometry is introduced (see section 7);
- REMO includes interpolation tools, which improve modelling of boundary conditions of the \( \beta \)-type and account, for monitored \( \phi \)-values of irregularly located observation wells;
- REMO relies mostly on line data; although, the ordinary pointwise ones can also be applied;
- the solution \( \phi \) of (1) is always represented by the following REMO superposition:

\[
\phi = \phi_s - d
\]  

where \( \phi_s \) is the conditionally "undisturbed" solution if \( \beta_w = 0 \) (no pumping wells are active); \( d \) is the drawdown vector when \( \beta_w \neq 0 \) and all other boundary conditions are nullified (\( \psi = 0, \beta_{in} = \beta_{out} = \beta_{sh} = 0 \)). Luckily, \( d \) can be computed even if no numerical values of the other boundary conditions, but \( \beta_w \), are available.

It follows from the above list that aquifers in REMO are always kept conditionally confined. If necessary, \( A \) of (1) should be corrected when under the impact of \( d \), considerable changes of the transmittivity \( a_{xy} \) of (2) take place, because then the saturated thickness of the corresponding aquifer decreases.

The REMO system is convenient for a modeller to calibrate HM, as it is done in a dialogue "man - computer": even for large HM (\( N \sim 10^5 \)), the processing time is about only tens of seconds and each \( k \) or \( m \) map of (2) can be re-adjusted on-line. For the first stage of calibration or for simple cases, constants can be used, instead of these maps.

5 INTERPOLATION OF DATA AND THE GDI PROGRAM

Even under an idealistic assumption that initial data contain no errors, the result of digital mapmaking may be wrong due to inapt interpolation methods used. This problem is only scantily mentioned in manuals on interpolation.

For the \( z, k, \beta \)-maps, interpolation surfaces represent geometrical images. Their quality is described by the residue of values (difference between the initial data and interpolated values). Naturally, this residue is minimal, at areas where the initial data are located.

On the other hand, modellers often neglect the notable fact that any initial data behave like sources of a formal mass with respect to the interpolated surface. This feature does no harm for the quality of the above-mentioned \( z, k, \) and \( \beta \)-maps, but it forbids direct use of initial data for making the \( \phi \)-maps of (1). These data may serve, as calibration targets only. In practice, this principal restriction is often ignored, and observed piezometric heads are incorrectly applied for direct interpolation. Thoughtless use of conventional interpola-
tion methods may produce unforeseen, hardly detectable errors. In more details, this aspect is considered below.

Initially, for creating the maps of (2), the EMC team managed to apply the wide-known interpolation methods: Criging, Minimal Curvature, Inverse Distance, etc. included in SURFER [3]. Unluckily, these methods sometimes provided evidently wrong results. For example, if an $m$-distribution was highly irregular and discontinuous, negative thicknesses appeared, even if the input ones were strictly positive [1]! It was understood that this unexpected failure was due to the following principal hindrances of these methods [14, 31]:

- interpolated results did not hold the maximum/minimum principle towards initial data applied;
- the interpolation surface did not carry a minimal energy;
- initial data were often overruled by practically uncontrollable algorithms applied for smoothing of the interpolation result; for example, the $m = 0$ areas were specified by dense zero initial data; perhaps, for the sake of the smoothness, some part of these data, during interpolating were forcefully changed for the $m < 0$ ones [1]; in general, errors of such kind are hard to detect.

Because of these drawbacks, the above mentioned conventional methods cannot provide strictly controllable interpolation results, even if dense initial data are applied. For this reason, the GDI program has been developed. Formally, it provides the interpolation surface $\sigma$ as the numerical solution of the following associated 2D-boundary problem, on the $xy$-grid of (1):

$$\partial(\lambda * \partial \sigma / \partial x) / \partial x + \partial(\lambda * \partial \sigma / \partial y) / \partial y = 0,$$

(4)

$$V \sigma = - G_{\sigma} \sigma_{w}, \quad V = V_{xy} - G_{\sigma}$$

(5)

where (5) is the algebraic equation system, applied to approximate the problem (4); the matrices $V_{xy}, G_{\sigma}$ represent, correspondingly, the horizontal links $v_{xy}$ of the interpolation plane, the elements of this plane $g_{\sigma}$ which connecting nodes of the $xy$-grid of HM with the boundary conditions $\sigma_{w}$ (initial data $\sigma_{o}$ of interpolation are used there); $\lambda = \lambda(xy)$ of (4) is the variable parametre, representing the formal "permeability" $k_{\sigma}$-map which gives the values $v_{xy}$ of $V$:

$$v_{xy} = \lambda(xy) = k_{\sigma}(xy)$$

(6)

where the $xy$-coordinate is given for the topological centre of the link $v_{xy}$.

The system (5) represents the 2D version of (1) where $\beta = 0$, and no concept of a layer thickness is applied ($m_{\sigma} = 1$). Due to this similarity, it was possible to apply for (5) the 2D-version of the REMO solver program (Nr 8).

As the fundamental feature of (4), $\sigma$ ever holds the both maximum/minimum and minimal energy principles. By applying the parametre $\lambda(xy)$, one can control the shape of $\sigma(xy)$. In areas where $\lambda = 1.0$, pointwise $\sigma_{w}$ usually produce sharp maximums. If $\lambda >> 1$ then such maximums become flat. Due to changeable $\lambda(xy)$, it is possible to modify individually the "strength" for each initial data source.

The GDI program mostly applies various line data as initial ones, because they are much more informative than few pointwise measurements 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, which dissects the $xy$-grid area, if necessary.

The GDI program is mainly applied in the sequential mode. During the current interpolation step, new information is applied, but the results of the previous step serve, as the base; the number of the steps is not limited. The mode is very effective if complex surfaces should be created as a result of natural geological and/or industrial scenario, which alters the simple initial shape into the complex one. In this way, the 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. This feature of GDI makes calibration of HM much easier.

The reported approach is focused on minimizing of GDI input data. It cardinaly differs from the one followed by a painter whose finished picture can be formally interpreted, as an interpolation result based on an immerse, hardly controllable set of initial data.
6 BOUNDARY CONDITIONS AND THE GROUND SURFACE ELEVATION MAP

On the surface of HM, applications of the fixed boundary flows $\beta_{\text{inc}}$, $\beta_{\text{bec}}$, and $\beta_{\text{sh}}$ of (1), must be avoided because they may cause the following undesirable side effects:

- considerable solution errors appear, because no verifiable field data are available about real distributions of these flows; this is especially true if large regional HM should be created;
- any $\beta$-surface considerably distorts the depression cone $d$ caused by $\beta_{\text{sh}}$ (the values of $d$ become larger than they should be);
- all $\beta$-surfaces worsen the convergence of any iterative solver program of (1);
- sensitivity of (1) towards possible errors will increase.

Fortunately for HM, the fixed flows can be always substituted for the more reliable computed ones $\beta_{\text{comp}}$ which also improve a work of any solver program. The changes $\beta_{\text{bec}} \rightarrow \beta_{\text{sh}}$, $\beta_{\text{bec}} \rightarrow \beta_{\text{sh}}$ are conventional [17]. However, the condition $\psi_{\text{sh}}$ for the HM shell should be treated unusually (see section 7) [16].

For infiltration $\beta_{\text{in}}$, the transformation $\beta_{\text{in}} \rightarrow \beta_{\text{sh}}$ is special. It always considerably improves HM, because the map $z_0 = \psi_{\text{sh}}$ is applied, as the boundary condition, and the aeration zone $\psi_{\text{aer}}$ (unsaturated part of the unconfined $q$ aquifer) is treated 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 $k_{\text{aer}}$ of the $\psi_{\text{aer}}$ zone can be apprised by applying the mean annual permeability $k_{\text{rm}}$:

$$k_{\text{rm}} = h_{\text{aer}} / \int k_{\text{aer}}^{-1} dh_{\text{aer}}, \quad k_{\text{aer}} = k_{\text{rm}} k_q$$

and the van Genuchten’s (vG) capillary model (8) for any unsaturated soil [19]. In (7), $0 \leq k \leq 1$ is the current relative permeability; $h_{\text{aer}}$ is the thickness of the zone, $0 \leq h_{\text{aer}} \leq h_{\text{aer}}$; $k_q$ is the permeability of the $q$ aquifer. Just below the ground surface of the recharge area, $k_q$ diminishes due both to evaporation processes and an impact of the capillary curve $S = S(h_q)$ there; $0 \leq S \leq 1$ is the normalized soil water content. The following formula:

$$k_q = S^{0.5} (1-(1-S^{1/\alpha})^\mu)^2, \quad S = (1 + (\alpha h_q)^{1/(1-\mu)})^{-\mu}$$

enables to estimate $k_q$. In (8), the relationship $S = S(h_q)$ is the kernel of the vG model where $\alpha$ and $\mu$ are its control parameters. If $S \sim 1$ then $k_q \sim 1$ (discharge areas); in the recharge areas: $S \ll 1$, $k_q$ is small, and the $\psi_{\text{aer}}$ zone behaves like an aquitard if its mean annual state is considered.

When $\psi_{\text{sh}}$ is applied, the flow $\beta_{\psi_{\text{in}}}$ passes through the aeration zone:

$$\beta_{\psi_{\text{in}}} = G_{\text{aer}} (\psi_{\text{sh}} - \phi_q), \quad g_{\text{aer}} = k_{\text{aer}} h_{\text{aer}} \geq 0$$

where $\phi_q$ is the computed head (subvector of $\phi$) for the $q$ aquifer; $G_{\text{aer}}$ (diagonal submatrix of $G$) contains the vertical ties $g_{\text{aer}}$ connecting $\psi_{\text{sh}}$ with $\phi_q$. The expression (9) reflects the usual support of HM when the $\psi$-condition is applied. The $\beta_{\psi_{\text{in}}}$ distribution is also handy for the HM calibration - both, as its tool ($g_{\text{aer}}$ variable) and target (some observed data for $\beta_{\text{in}}$ and $\phi_q$ are available). The calibrated $\beta_{\psi_{\text{in}}}$ 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 $\phi$-distribution is obtained". In reality, $h_{\text{sh}}$ is variable:

$$\begin{align*}
\text{if } \beta_{\psi_{\text{in}}} & \geq 0, \quad h_{\text{sh}} = \psi_{\text{sh}} - z_q - m_q, \quad m_q = \phi_q - z_q; \\
\text{if } \beta_{\psi_{\text{in}}} & < 0, \quad h_{\text{sh}} = \Delta = 2 \text{ cm}
\end{align*}$$

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

As it follows from (10), real $h_{\text{sh}}$ and $m_q$ are unknown beforehand and should be obtained from the calibrated system of (1), if the actual geometry is important; for example, when HM is applied as a driver for modelling contaminant transport processes in groundwater.
In HM, the \( q \) aquifer is regarded as conditionally confined, and the initial try for its transmittivity distribution \( a_q \) is, as follows:

\[
a_q^{(0)} = c_q^{(0)} k_q^{(0)} m_q^{(0)}, \quad m_q^{(0)} = \psi_{rel} \cdot z_q + \Delta
\]

where \( c_q^{(0)}, k_q^{(0)}, \) and \( m_q^{(0)} \) are the initial distributions, correspondingly, of the correction factor (dimensionless), the permeability, and the full thickness for the \( q \) aquifer. Until HM has not been calibrated, \( m_q^{(0)} \) remains unchanged; the small constant \( \Delta \) of (10) substitutes a thickness of the \( m = 0 \) areas also for all kinds of discontinuous or fictitious layers of HM. Due to smallness of \( \Delta \), the HM geometry is not really distorted, even if many of such layers are present in HM. There \( \Delta \) serves the following tasks:

- controls values of elements \( a_q \) (a \( q \) of (11)) and \( a_t \) (\( g_{aer} \) of (9)) via the proper choice of the corresponding permeability \( k_q \) (\( k_t \) of (11)) and \( k_q \) (\( k_{aer} \) of (9)) distributions;
- prevents an occurrence of a negative thickness for a layer, due to computational round off errors of its top and bottom surfaces (\( \psi_{rel} \) and \( z_q \) for (11)).

The value of \( \Delta \) may be chosen rather arbitrary. It must be small enough not to disturb the HM geometry of multilayered systems. For discontinuous aquitards, \( \Delta \) must cause large values of the elements \( a_z \).

Generally, the factor \( c_q \) is:

\[
c_q = (m_q^{(0)} - h_{aer}) / m_q^{(0)} = \text{var} \leq 1.0.
\]

If \( h_{aer}^{(0)} = \Delta \) (see (13)) then \( c_q^{(0)} = 1.0 \).

For \( g_{aer}^{(0)} \), the general formula (9) must be specified, because instead of the unknown variable \( h_{aer} \), constant \( h_{aer}^{(0)} = \Delta \) should be applied temporarily elsewhere:

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

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

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

After \( k_q^{(0)} \rightarrow k_q^{(1)}, k_{aer}^{(0)} \rightarrow k_{aer}^{(1)} \), the first calibrated solution \( \psi_{rel}^{(1)} \) is obtained, and the distributions \( h_{aer}^{(1)} \) and \( m_q^{(1)} \) can be specified, to introduce the necessary real HM geometry of (10).

The real geometry has no impact on numerical values of \( a_q^{(1)} \) and \( g_{aer}^{(1)} \). It uses only their "real" ingredients, as follows:

\[
a_q^{(1)} = k_q^{(1)} m_q^{(1)}, \quad k_q^{(1)} = k_q^{(0)} m_q^{(0)} / m_q^{(1)},
\]

\[
g_{aer}^{(1)} = k_q^{(1)} h^2 / h_{aer}^{(1)}, \quad k_q^{(1)} = c_{aer}^{(0)} k_{aer}^{(1)} h_{aer}^{(1)} / \Delta
\]

where \( m_q^{(0)} \rightarrow m_q^{(1)}, \Delta \rightarrow h_{aer}^{(1)}, \) and \( k_q^{(1)} \rightarrow k_q^{(0)}, k_{aer}^{(1)} \rightarrow k_{aer}^{(0)} \). Now from (10), one can obtain the final \( z_q \) map that is applied, as the input for the GV system.

Recently ([11]), project Nr 8, the treatment of \( \beta_{q,in} \) has been improved. The distributions \( m_q^{(1)}, h_{aer}^{(1)} \) are applied for correcting the factors \( c_q^{(1)}, c_{aer}^{(1)} \):

\[
c_q^{(1)} = m_q^{(1)} / m_q^{(0)},
\]

\[
c_{aer}^{(1)} = \begin{cases} \sigma^{(1)} = (h_{aerm} / h_{aer}^{(1)})^u \quad \text{if} \quad h_{aer}^{(1)} > h_{aerm}, \\ c_{aer}^{(0)} \quad \text{if} \quad h_{aer}^{(1)} \leq h_{aerm}. \end{cases}
\]

where \( 1 > u > 0 \) is the parameter used to control \( c_{aer}^{(1)} \) for the recharge areas, if \( h_{aer}^{(1)} > h_{aerm} \). If \( u = 1 \) then the \( \beta_{q,in} \) only slightly depends on \( \psi_{rel} \). Currently, the value \( u = 0.75 \) has been accepted as an optimal choice.

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

\[
a_q^{(1)} = c_q^{(1)} k_q^{(1)} m_q^{(0)}, \quad g_{aer}^{(1)} = c_{aer}^{(1)} k_{aer}^{(1)} h^2 / \Delta.
\]
In (14), \( k_q = k_q^{(i)} \) and \( k_a = c_{zcc}^{(i)} k_{scc}^{(i)} h^2 / \Delta \). The reported innovation has considerably reduced the effort spent to calibrate \( \beta_{\psi_{rel}} \).

When the \( \psi_{rel} \) map is applied, the HM results are characterized by:
- the surface \( \varphi_{sh} \) automatically follows main geometrical features of \( \psi_{rel} \), because \( g_{scc} \) interlinks both surfaces; for humid areas, this natural phenomenon will always be present;
- it follows from (9) that components of \( \beta_{\psi_{in}} \) respond correctly to a depression cone \( d \) of (3) caused by \( \beta_{in} \) (\( \beta_{\psi_{in}} \) increases if \( d \) enlarges); when fixed \( \beta_{in} \) is used, this important natural response cannot be automatically accounted for;
- HM provides the \( \beta_{\psi_{in}} \) distribution, which defines the infiltration intensity and clearly indicates the areas of discharge and recharge.

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

In practice, even the crude attempt (11) and (13) provides surprisingly good results for complex regional HM [1, 4]. In these cases, it is likely, no HM can be obtained by conventional approach requiring use of fixed \( \beta_{in} \). The reasons for such pessimism are:
- 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 fixed \( \beta_{in} \); computed \( \varphi_{sh} \) often occurs above the ground surface \( \psi_{rel} \) (an impossible situation for an unconfined aquifer), because for fixed \( \beta_{in} \), \( \varphi_{sh} \) does not follow \( \psi_{rel} \).

The method of modelling the mean annual infiltration can be run by any HM system, for example, by the GV program. However, no regimes of unconfined aquifers must be used there, otherwise the MODFLOW code involved may ruin HM, especially, if HM contains discontinuous layers [9]. Then the destruction of HM is inevitable, due to irreparable, automatic annihilation of "dried" (\( m_q = 0 \)) 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 \( \psi_{rel} \)-map, in the MODFLOW code environment, the surface \( rel \) should be specified, as a formal thin aquifer (\( \Delta_{rel} = 2 \) cm).

7 THE HM SHELL APPLIED FOR INTERPOLATION OF BOUNDARY CONDITIONS

Special problems arise when the difference between computed \( \varphi \) values (\( \text{grad} \varphi \)), belonging to interlinked aquifers becomes very small. It happens, in areas of hydrogeological windows (\( m = 0 \)) of discontinuous aquitards, where the elements \( a_z \) of (2) have very large values (theoretically, \( a_z \to \infty \) if \( m = 0 \)). The expected value of (\( \text{grad} \varphi \)) is given by the general formula:

\[
(\text{grad} \varphi)_z = \beta_z / a_z
\]

where \( \beta_z \) is the computed limited flow passing through \( a_z \).

On an intersection of the window with the shell, the \( \psi_{sh} \)-values behave similarly, as the ones of \( \varphi \). In complex practical cases, for example [1], the non-existent parts of aquitards constitute a multi-tiered system where aquifers are also absent (\( a_{sh} = 0 \)). It was necessary to find a method providing reliable \( \psi_{sh} \) for the above reported case when at numerous places, on the HM shell, (\text{grad} \varphi)_z \approx 0 \) was expected. No conventional software could produce \( \psi_{sh} \) without disrupting the HM space continuity. The problem was solved numerically by introducing a multiplier constant (\( u_{sh} = 10^3 - 10^4 \)), to enlarge artificially, the values \( g_{syr}, g_{sy}, g_{z} \) of links connecting nodes of the shell. The converted shell then acts like an almost ideally conducting shield which computes missing values of \( \varphi \), as a special portion of the solution \( \varphi \) in its nodes where no initial boundary \( \varphi \)-conditions are fixed. Due to such a converted shell, both fixed and computed head values on its surface behave as the \( \varphi \)-type conditions towards the inside of the HM body.

One should not involve the shell into water balance calculations of HM, because flows here are \( u_{sh} \)-fold larger than the normal ones. To include the shell into these balances, its normalization must be done, as follows:
- final \( \psi_{sh} \) is applied, as the fixed one;
- normal \( g_{syr}, g_{z} \) are used instead of the enlarged ones.

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For controlling features of the GDI program [14], transforming elements of the shell was also applied. In GDI, two characteristic distinct 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 linear interpolator. If one wants to use a constant boundary value, it must be fixed only in one arbitrary chosen point of the boundary. When nothing is fixed there then some mean computed boundary value appears. If \( u_{sh} = 0.5 \) then, in the fragments where no initial data are specified, the boundary acts like an impervious one (isolines of the interpolated parameter are orthogonal to the border line). Both characteristic \( u_{sh} \) values are applied, because they enable modify results of the GDI-interpolation in a wide range.

The converted shell enables to create HM of utmost complexity, because high quality of boundary conditions is granted automatically. This useful novel approach can be applied in all kinds of modelling programs developed for building of HM.

8 DEALING WITH THE ZONE SCHEME PROBLEM

For the first generations of digital computers, any rational idea of memory saving was supported. The zone scheme is a survivor from this time. It is shown in this section that the scheme has become a serious hindrance, and some effort must be spent to neutralize its side effects, occurring even in the GV program.

In the past, only simple HM were created (mostly for 2D areas with coarse \( k \) and \( m \) distributions). No computer-based tools were available for data interpolation and a modeller was the main force of creating HM. Under these conditions, the first modelling software originated, and the zone scheme was introduced. It was based on the following reasonable assumptions:

- rather small numbers \( N_k, N_m << N \) of constants were needed to describe the course initial \( k \) and \( m \) distributions, because within large areas of the HM grid (zones), the \( k \) and \( m \) parameters were equal due to a crude staircase type approximation used;
- a modeller was able to specify manually the relationship between these zones, as geometrical images represented by polygons, and the corresponding constant values of \( k \) and \( m \); no special interpolation programmes were needed to solve such a simple task;
- a considerable memory saving was possible, because only a small list containing the addresses of the HM grid nodes, corresponding with the zone constants of \( k \) and \( m \), was stored.

Due to obvious advantages of this approach, the scheme was widely accepted and applied both by modelers and developers of the modelling programs. Today, the zones are uncritically used even by the advanced modeling software such as GV, in spite of the fact that none of the three above assumptions favoring the zone scheme is valid any longer:

- the basic condition \( N_k, N_m << N \) is not true for modern HM; moreover, high quality \( k \) and \( m \) distributions can be created beforehand by special interpolation tools where \( N_k = N_m = N \);
- if \( N_k, N_m \) are large, a modeller cannot create manually veritable data maps; especially, when one deals with the computed \( k/m \) leakance distribution;
- there is no need to save a computer memory.

If a modern modelling program incorporates the zone scheme, the following problems are evident:

- the data prepared for HM by an external software (interpolation, calibration, etc.), or computed within the modelling program (for example, the leakance \( m/k \)), may inadvertently get distorted, even ruined, due to bad tuning of the data converter module transforming such an information into the zone memory representation or backwards;
- according to the zone scheme, a modeller fully participates in interpolating of the HM data; and the risk of numerous human, hardly detectable errors becomes high;
- the Windows system, used in the GV program for graphing zone polygons interactively on the computer screen, does not provide them as open data files for independent tools of interpolation; because of this mishap, any result based on a such a visual representation, is like a work of art, which can never be repeated in all details, even by its author;
- as a coarse approximation, the zone scheme becomes awkward, if one tries to run it, as a numerical method; an enormous amount of data is needed to describe \( N_k \) or \( N_m \) tightly coordinated polygons, which must be used to interpolate jumplike changes of \( k \) and \( m \) parameters, accordingly, between neighboring zone areas of the HM grid;
- the forward and backward conversion processes for zones are time consuming.
Because of the above problems, it is not recommended to use any zone-based technologies. They can be avoided, even in the GV environment, if the existing zone conversion modules are rightly tuned, or the new ones are developed.

The zone converter transforms data into the numbers of zones and backwards, as follows:

\[
\begin{align*}
    s_j &= s_0 + \Delta_0 j, \\
    \Delta_0 &= (s_n - s_0) / (1 + i_n - i_1), \\
    j &= 1 + i_j - i_1, \\
    n &= 1 + i_n - i_1, \\
    j &= 1, 2, ..., n
\end{align*}
\]  

(19)

where \(s_0, s_j, s_n\) are start, current, and end values, respectively, of the interval \((s_0, s_n)\) to be converted; \(i_1, i_j, \text{ and } i_n\) are start, current and end numbers of \(n\) zones applied; \(\Delta_0\) is the interpolation increment; \(j\) is the current number used to compute \(s_j\).

The relative error \(\delta_j\ [%]\) of (19) is given by the ratio:

\[
\delta_j = 10^2 \Delta_0 / s_j, \quad \delta_{\text{max}} = 10^2 \Delta_0 / s_0, \quad \delta_{\text{min}} = \delta_{\text{max}} s_0 / s_n
\]  

(20)

If the ratio \(s_n / s_0 >> n\) then the interval \((s_0, s_n)\) should be covered by \(v\) subintervals where different \(\Delta_0^{(t)}\) \((t = 1, 2, ..., v)\) must be applied, in order to keep the error \(\delta_{\text{max}}\) under control. Let us consider the following typical example of the leakance \(k/m\) data: \(s_0 = 10^{-9}; s_n = 10; s_n / s_0 = 10^{10} >> n = 10^5\). If one tries to code these data, in a single interval, then \(\delta_{\text{max}} = 10^{12} %\) ! It means that small values of \(s_j\) will be inevitably lost, during the zone conversion. In [4], the error \(\delta_{\text{max}} = 0.9 %\) was insured by introducing \(v = 10\) decade (1:10) subintervals, as shown in Table 3. For each subinterval, \(10^5\) zones were used.

TABLE 3. Zone coding by applying decade subintervals

<table>
<thead>
<tr>
<th>t</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i_1)</td>
<td>1</td>
<td>1001</td>
<td>2001</td>
<td>3001</td>
<td>4001</td>
<td>5001</td>
<td>6001</td>
<td>7001</td>
<td>8001</td>
<td>9001</td>
</tr>
<tr>
<td>(i_n)</td>
<td>1000</td>
<td>2000</td>
<td>3000</td>
<td>4000</td>
<td>5000</td>
<td>6000</td>
<td>7000</td>
<td>8000</td>
<td>9000</td>
<td>10000</td>
</tr>
<tr>
<td>(s_0)</td>
<td>(10^{-9})</td>
<td>(10^{-5})</td>
<td>(10^{-3})</td>
<td>(10^{-1})</td>
<td>(10)</td>
<td>(9 \times 10^{-12})</td>
<td>(9 \times 10^{-11})</td>
<td>(9 \times 10^{-10})</td>
<td>(9 \times 10^{-9})</td>
<td>(9 \times 10^{-8})</td>
</tr>
<tr>
<td>(\Delta_0)</td>
<td>(9 \times 10^{-10})</td>
<td>(9 \times 10^{-12})</td>
<td>(9 \times 10^{-14})</td>
<td>(9 \times 10^{-16})</td>
<td>(9 \times 10^{-18})</td>
<td>(9 \times 10^{-20})</td>
<td>(9 \times 10^{-22})</td>
<td>(9 \times 10^{-24})</td>
<td>(9 \times 10^{-26})</td>
<td>(9 \times 10^{-28})</td>
</tr>
</tbody>
</table>

The decade scheme is customary for a modeller who must manually enter Table 3 in a computer, in order to tune the zone converter module of the GV program. Other numerical systems, for example, the octal (1:8) and hexadecimal (1:16) ones may be useful if the converter is tuned automatically.

It is possible to improve considerably the result provided by Table 3, especially, when new automated converters are to be developed. Within a decade, the current error \(\delta_j\) evenly decreases from \(\delta_{\text{max}} = 0.9 %\) to \(\delta_{\text{min}} = 0.09 %\), and \(q = \delta_{\text{max}} / \delta_{\text{min}} = 10.0\) (see Fig.1).

![Figure 1](image.png)

**Figure 1.** Graphs of the current relative error \(\delta\) for the basic decade (1.00, 10.00); the graphs 1, 2 describe, correspondingly, the single decade and the one with two subintervals (1.00, 3.16), (3.16, 10.00). The notched graph of \(\delta\) turns into the horizontal \(\delta = 0.230\) when \(v = n = 1000\) (see Table 4).
The ratio \( q \) can be reduced \( 10^{1/v} \) fold if the decade (1.00, 10.00) is covered by \( v \) subintervals. Each subinterval includes \( n/v \) zones where \( n \) is the total number of zones applied for the interval. The tuning parameters for the converter are given by the following formulas:

\[
q = \frac{\delta_{\text{max}}}{\delta_{\text{min}}} = 10^{1/v}, \quad \delta_{\text{max}} = 10^{2(q - 1)v/n}, \quad s_0^{(i)} = q^{t-1},
\]

where \( s_0^{(i)}, \Delta_0^{(i)} \) are the start and increment values, accordingly, of the \( t \)-th subinterval. The graph of \( \delta \) contains \( v \) notches enveloped by the horizontals \( \delta_{\text{max}} \) and \( \delta_{\text{min}} \). The graphs for \( v = 1, 2 \) are shown in Fig.1. Numerical parameters, given by (2) when \( n = 10^3 \) are included, in Tables 4 and 5.

**TABLE 4.** Parametres for the first subinterval (\( t = 1 \)) of the decade (1.00, 10.00) coded by \( n = 10^3 \) zones in \( v \) subintervals

<table>
<thead>
<tr>
<th>( v )</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>10</th>
<th>20</th>
<th>100</th>
<th>1000</th>
</tr>
</thead>
<tbody>
<tr>
<td>( q = s_0^{(1)} )</td>
<td>10.000</td>
<td>3.162</td>
<td>2.154</td>
<td>1.778</td>
<td>1.259</td>
<td>1.122</td>
<td>1.023</td>
<td>1.002</td>
</tr>
<tr>
<td>( \delta_{\text{max}} % )</td>
<td>0.900</td>
<td>0.432</td>
<td>0.346</td>
<td>0.311</td>
<td>0.259</td>
<td>0.244</td>
<td>0.233</td>
<td>0.230</td>
</tr>
<tr>
<td>( \Delta_0^{(1)} \cdot 10^3 )</td>
<td>9.000</td>
<td>1.365</td>
<td>0.745</td>
<td>0.553</td>
<td>0.326</td>
<td>0.274</td>
<td>0.238</td>
<td>0.230</td>
</tr>
</tbody>
</table>

**TABLE 5.** Tuning parameters for the decade (1.00, 10.00) covered by \( n = 10^3 \) zones if \( v = 10 \)

<table>
<thead>
<tr>
<th>( t )</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
</tr>
</thead>
<tbody>
<tr>
<td>( s_0^{(1)} )</td>
<td>1.000</td>
<td>1.259</td>
<td>1.585</td>
<td>1.995</td>
<td>2.512</td>
<td>3.162</td>
<td>3.981</td>
<td>5.012</td>
<td>6.309</td>
<td>7.943</td>
<td>10.000</td>
</tr>
<tr>
<td>( \Delta_0^{(1)} \cdot 10^3 )</td>
<td>0.259</td>
<td>0.326</td>
<td>0.410</td>
<td>0.517</td>
<td>0.650</td>
<td>0.819</td>
<td>1.031</td>
<td>1.298</td>
<td>1.634</td>
<td>2.057</td>
<td>—</td>
</tr>
</tbody>
</table>

It follows from Tables 4 and 5 that the method based on (21) considerably reduces the parameter \( q \) and the error \( \delta_{\text{max}} \), as well. The case (\( v = 10; n = 10^3 \)) of Table 5 seems to be optimal, because its main characteristics (\( q = 1.259 > 1.002, \delta_{\text{max}} = 0.259 > 0.230 \)) are only slightly lower than the ones of the ultimate case (\( n = v = 10^3 \)). It follows from the above considerations that it is possible to introduce effective methods for tuning the converter module, in order to eliminate possible errors caused by the zone scheme.

### 9 CONCLUSIONS

The EMC team has dealt with complex practical projects and has developed new software tools, which are being applied in conjunction with the conventional ones, to perform these projects successfully. The following general ideas are supported by the team:

- model formulation, solving, and post-processing errors can be subdued if special software and methodology are focused on this purpose;
- involvement of people in routine processes, which can be run much safer by a properly designed software, should be reduced;
- various, highly effective special tools should be applied to create complex models, because no single system can cope with such a task.

Know-how reported in this paper may be useful for modellers dealing with the problem of creating hydrogeological models.

### REFERENCES


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Kopš 1993.gada, Rīgas Tehniskās universitātes Vides modelēšanas centra (VMC) speciālisti ir aktīvi piedalījušies speciālu programmatūru izstrādāšanā hidrogeoloģisko modeļu (HM) vajadzībām. Šie jaunie programmatūras līdzekļi tiek izmantoti kopā ar komerciālo programmatūru, lai risinātu praktiskas problēmas šīdens apgādes un pazemes ūdeņu dināmikas jomā. Tiek apskatīti VMC jaunie programmatūras līdzekļi un galvenie projekti, kuri izstrādāti ar to palīdzību.

Спальвиньш А., Шлангенс Я., Янбикис Р., Лаче И., Эглите И., Шкибелис В., Мачанс А. Новые технологии для моделирования гидрогеологических процессов.
Начиная с 1963 года Центр моделирования окружающей среды (ЦМОС) Рижского технического университета активно разрабатывает программные средства для построения гидрогеологических моделей. Новые средства были использованы совместно с коммерческими программами для решения практических проблем, которые связаны с добывчей питьевой воды и динамикой подземных вод. Рассматриваются новые программные средства, а также главные проекты в которых ЦМОС принимает участие.