

# THE NOGINSK DISTRICT (RUSSIA) CASE AS AN ILLUSTRATION OF NOVEL SIMULATION TECHNOLOGIES DEVELOPED FOR CREATING HYDROGEOLOGICAL MODELS

A. Spalvins, J. Slangens, R. Janbickis, I. Lace

Environment Modelling Centre, Riga Technical University, Latvia

L. Loukiantchikova

All-Russian Research Institute for Hydrogeology and Engineering Geology, Russia

E. Gosk

Geological Survey of Denmark and Greenland, Denmark

## Abstract

Since 1993, the team of the Environment Modelling Centre (EMC) of the Riga Technical University is being active in the field of developing methodologies and special software for creating hydrogeological models (HM). In this paper, these tools applied together with commercial ones are described, on the example of complicated HM created for the Noginsk District, Moscow Region, Russia. The model was obtained due to efforts of joined teams of EMC and the All-Russian Research Institute for Hydrogeology and Engineering Geology.

## 1. Introduction

This paper shows applications of special and commercial software tools used recently for creating Noginsk HM (see Table 1, Spalvins et al., 1999, Spalvins et al., 2000a, Spalvins et al., 2000c, Loukiantchikova et al., 2000, Gosk et al., 1999).

To elucidate the main problems associated with creation of this HM, it is necessary to discuss some mathematical procedures applied. The  $xyz$ -grid of HM is built of  $(h \times h \times h_z)$ -sized blocks ( $h$  is the block plane size;  $h_z$  is a variable block height). They constitute a rectangular  $(2s + 1)$  – tiered  $xy$ -layer system where  $s + 1$  and  $s$  are the number of aquifers and interjacent aquitards, accordingly. Its four vertical sides compose the shell of the HM grid. For Noginsk HM:  $h = 500$  m,  $s = 7$ , the model and grid sizes are, correspondingly,  $39$  km \*  $36$  km \*  $0.3$  km, and  $79 * 73 * 8 = 46,136$  nodes.

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

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

where the matrices  $A_{xy}$ ,  $A_z$ , and  $G$  represent horizontal links  $a_{xy}$  of aquifers (arranged in  $xy$ -planes), vertical ties  $a_z$  originated by aquitards, and elements connecting “free” nodes of the grid with the nodes for which the piezometric boundary conditions  $\psi$  are specified; in Noginsk HM, the  $\psi$ -distribution exists on the whole HM surface, and the source vector  $\beta$  contains only rates of the groundwater withdrawal;  $\beta_\psi$  is the computed flow passing through elements of  $G$ . The elements  $a_{xy}$ ,  $a_z$  (or  $g_{xy}$ ,  $g_z$  of  $G$ ) are computed, as follows:

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

where  $z_{i-1}$  and  $z_i$  are the elevation distributions of the top and bottom surfaces of the  $i$ -th geological layer;  $z_0$  represents the ground surface map  $\psi_{rel}$  with the hydrographical network (lakes, rivers, etc.) included;  $m = h_z$ ,  $k$  are elements of the digital  $m$ ,  $k$ -maps of computed thickness and permeability distributions of layers, respectively.

The set of the  $z_i$ -maps states the full geometry of HM. If, within some area,  $h_{z_i} = 0$  then the  $i$ -th layer is discontinuous. Noginsk HM includes 7 discontinuous layers, and this feature makes creating of this model difficult (Gosk et al., 1999).

## 2. General scheme. Software applied

The process of making Noginsk HM conditionally contains the following stages:

- scanning hard copies of necessary maps, in order to convert them into electronic images;
- digitizing the electronic images of maps defining the geological  $z$ -surfaces, eq. (2) and preparation of the full set of these surfaces; this was the most difficult and time-consuming part of the definition of the Noginsk HM;
- construction of  $k$ -,  $\beta$ - and  $\psi$ -distribution maps; applying of these maps for HM calibration; the modelling system REMO (Spalvins et al., 1996) is applied at this stage, and all calibrated HM results become available for further utilization;
- the contaminant mass transport was modelled by the Groundwater Vistas (GV) system (Environmental simulations, 1997); the HM data for GV were prepared by REMO.
- the SURFER program (Golden Software, 1997) was 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 (McDonald & Harbaugh, 1988) and interpolation modules of SURFER) turned out to be insufficient for handling of practical cases involving complex hydrogeological systems (Atruskievics et al., 1994). Even today, many of the modern modelling programs (like GV) are including some outdated principles inherited of the era of slow computers: the zone scheme for saving memory (Spalvins & Janbickis, 2000); the pure  $\beta$ -condition applied, as the infiltration flow  $\beta_m$  on the HM top (Spalvins, 2000); unnecessarily strong human involvement (Spalvins et al., 1999, Spalvins et al., 2000c), etc. Unfortunately, these principles cause serious trouble, when one tries to apply the GV system for preparing Noginsk HM in a straightforward manner (Gosk et al., 1999).

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 affined program, even the commercial one. The column "Related programs" 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.

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

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 (Spalvins et al., 2000a, Spalvins et al., 2000c).

The remarkable GDI-results are also due to extensive use of various line data (isolines, geological boundaries and profiles of sections, long lines of rivers, etc) as input for GDI. These are computed by the CRP program, at intersections (cross-points) of lines (carriers) with the HM grid. The novel version of CRP insures high quality of coordinates and values of data, at the cross-points (Slangens & Spalvins, 2000).

Nr	Name of program or method and its function, (reference)	Related software
1	Program REMO, modelling and calibration of (1), (Spalvins et al., 1996)	GV, SURFER
2	Program GDI, creating interpolated data surfaces for (1), (Spalvins & Slangens, 1994)	REMO, GV, SURFER
3	Program CRP, preparing line data and joining them with the HM grid, (Slangens & Spalvins, 2000)	GDI
4	Program CRS, preparing line data of geological sections, (Lace & Spalvins, 2000)	CRP
5	Program INT $\beta\phi$ , interpolates $\beta$ and $\phi$ values from irregularly located wells to nodes of the HM grid and backwards, (Lace et al., 1995)	REMO
6	Program INT $\beta$ , interpolates $\beta$ values from irregularly located wells to nodes of the HM grid, (Gosk et al., 1999)	GV
7	Program GVR, creates images of vertical cross sections of HM results along any line chosen, (Spalvins et al., 1996)	REMO
8	Program NFCG, solves the system (1), (Janbicka et al., 1993)	REMO
9	Method of using the ground surface elevation map, as the $\psi$ -distribution, on the HM top, (Spalvins, 2000)	REMO, GV
10	Method of using the HM shell, as an interpolation device of the $\psi$ -distribution, (Spalvins, et al., 2000b)	REMO, GV
11	Method of tuning zone converter modules, (Spalvins & Janbickis, 2000)	GV

Table 1. Programs and methods developed by the EMC team for creating HM.

The INT $\beta\phi$  program considerably improves accuracy of REMO results in a following way:

- boundary  $\beta$ -values of irregularly located wells are interpolated to four nearest nodes of the HM grid; (GV roughly moves the  $\beta$ -value to the one nearest node!);
- $\phi$ -values are computed at irregularly (with respect to the HM grid) sited observation wells in order to increase accuracy of HM calibration.

The subsidiary INT $\beta$  program considerably improves the  $\beta$ -distribution for the GV code by applying the REMO interpolated  $\beta$ -values, as the formal production wells, at nodes of Noginsk HM (Gosk et al., 1999).

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 erroneous (Spalvins et al., 2000a).

As the REMO solver, the NFCG program is a robust, reliable tool. No adjustments of its regimes are required from a modeller.

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 the next section).

To prevent damage of data files imported into the GV system, the method Nr 11 of tuning the GV zone converter was developed.

It follows from Table 1 that, for Noginsk HM, many tools developed by EMC has been applied. Even some new ones have been made and used.

### 3. The landscape elevation map as the boundary condition. The HM shell as an interpolation device

Conventionally, the fixed flow  $\beta_{in}$  of the  $\beta$ -type is applied for specifying infiltration through the HM top surface. For regional Noginsk HM, such an approach would never produce good results, and the computed flow  $\beta_{\psi in}$  was applied instead of the fixed one (method Nr 9).

The landscape elevation map  $\psi_{rel}$ , as the  $\psi$ -type boundary condition for (1), was successfully applied, since 1995. This method assumes that the  $\psi_{rel}$  surface is piezometric, and the aeration zone *aer* (part of unconfined aquifer *q*) behaves like an aquitard, according to the capillary van Genuchten's (VG) model for the unsaturated soil (Genuchten, 1980). The VG model predicts the distinct permeability values:  $k_{aer} \sim 10^{-2} - 10^{-3}$  [m/day] and 1 - 10 [m/day], accordingly, for the areas of descending (infiltration) and ascending (discharge) flows of the aeration zone. The ascending flows are caused mostly by elements of the hydrographical network (rivers, lakes etc.) included in  $\psi_{rel}$ . Through the aeration zone, passes the flow  $\beta_{\psi in}$  (automatic replacement of  $\beta_{in}$ ):

$$\beta_{\psi in} = G_{aer} (\psi_{rel} - \varphi_q), \quad g_{aer} = k_{aer} h^2 / h_{aer} \geq 0 \quad (3)$$

where  $\varphi_q$  is the computed head (subvector of  $\varphi$ ) for *q*;  $G_{aer}$  (diagonal submatrix of  $G$ ) contains the vertical ties  $g_{aer}$  connecting  $\psi_{rel}$  with  $\varphi_q$ ;  $h_{aer}$  is the thickness distribution of the *aer* zone. The expression (3) reflects the usual support of HM, when the  $\psi$ -condition is applied. The  $\beta_{\psi in}$ -distribution is also helpful for the HM calibration - both, as its tool ( $g_{aer}$  variable) and target (some observed data for  $\beta_{in}$  and  $\varphi_q$  are available). The calibrated representation (3) must be achieved iteratively under the following important limitation used by EMC: "due to complexity of any geometrical change of HM, the geometry must remain fixed, until the final calibrated  $\varphi$ -distribution is obtained". Really, the thicknesses  $h_{aer}$  and  $h_q$  (saturated part of *q*) are variable, and this feature is accounted for by the method discussed in (Spalvins, 2000). In practice, even the crude  $k_{aer}$ -distribution (only two distinct  $k$ -values used) provides surprisingly good results for Noginsk HM (Gosk et al., 1999). The above method can be run by any HM system, for example, by the GV program

On the HM shell, difficulties of interpolating the boundary  $\psi$ -distribution arise when aquitards are discontinuous. Then elements  $a_z$  ( $g_z$ ) of (2) have large values (theoretically  $a_z \rightarrow \infty$  if  $h_z = 0$ ) and the vertical gradient of  $\varphi$  (or  $\psi$ ) becomes very small, in areas where  $h_z = 0$ . In Noginsk HM, the shell surface intersects with such areas, at numerous places. For this situation, no modeller is able to produce manually the proper  $\psi$ -distribution on the HM shell.

According to (Spalvins et al., 2000b), the above problem was solved numerically (method Nr 10) by introducing a multiplier constant  $u_{sh} = 10^3 - 10^4$ , to enlarge artificially the values  $g_{xy}$ ,  $g_z$  of links connecting nodes of the shell. The converted shell acts like an almost ideally conducting shield, which automatically interpolates missing values of  $\psi$  as a special portion of  $\varphi$ , in the nodes of the shell where no initial boundary conditions are fixed.

The above innovation has been applied by EMC, since 1995. It overcomes the difficult numerical problem caused by hydrogeological windows frequently found in the aquitards.

## Conclusions

The HM has been created for the Noginsk District. It serves as a framework for obtaining credible prognoses about available groundwater resources and trends of contaminant migration. The results obtained by the HM were used to prepare vulnerability maps of the District.

To obtain reliable HM results for complex practical cases, novel tools based on the following general ideas have been developed:

- number and severity of errors occurring during model formulation, solution of the problem and post-processing of the results can be reduced if special software and methodology is focused on this problem;
- involvement of people in routine processes, which can be managed by properly designed software, should be reduced;
- it is feasible to apply variety of highly effective specialised tools for creating complex HM, because no single system can cope with such a task.

We hope that our experience reported here would be useful for modellers dealing with hydrogeological models.

Noginsk HM was the part of the project *Groundwater Contamination and Remediation, Noginsk District, Moscow Region*. It was carried out with a financial support of the Danish EPA in the period May, 1998 to May, 2000 under the agreement by the Geological Survey of Denmark and Greenland and the All-Russian Research Institute for Hydrogeology and Engineering Geology.

## References

- ATRUSKIEVICS J., JANBICKIS R., KRUTOFAL T., LACE I., LEVINA N., SLANGENS J., SPALVINS A., VIKSNE, Z., (1994) Computer Based Regional Hydrogeological Model "Large Riga", *Boundary Field Problems and Computers, Proc. of Latvian - Danish Seminar on "Groundwater and Geothermal Energy"*, Riga – Copenhagen, **2**, 35, 203-224.
- Environmental Simulations, Inc., (1997) *Groundwater Vistas, Guide to using*.
- Golden Software, Inc., (1997) *Surfer 6.0 for Windows, User's manual*.
- GOSK E., SPALVINS A., VARTANYAN G. (eds.), (1999) Hydrogeological and Contamination Transport Models for Noginsk District, Moscow Region, *Report on Sub-contractor Agreement within the Project: Groundwater Contamination and Remediation in Noginsk District, Moscow Region*, Riga – Moscow.
- JANBICKA A., SPALVINS A., SLANGENS J., (1993) Implementation of the Nested Factorization Conjugate Gradient Method on a Spatial Grid, *Boundary Field Problems and Computers, Numerical Simulation for Hydrogeology*, Riga, **34**, 35-41.
- LACE I., SPALVINS A., (2000) Incorporating Geological Sections in Hydrogeological Models, *Scientific Proc. of Riga Technical University in series "Computer Science", Boundary Field Problems and Computer Simulation*, Riga, **4**, 42, 41-46.
- LACE I., SPALVINS A., SLANGENS J., (1995) Algorithms for Accounting Groundwater Discharge in the Regional Hydrogeological Model and Interpolation of Simulation Results at Observation Wells, *Boundary Field Problems and Computers, Proc. of International Seminar on "Environment Modelling"*, Riga – Copenhagen, **1**, 36, 201-216.

- LOUKIANTCHIKOVA L., GOSK E., SPALVINS A., JANBICKIS R., LACE I., (2000) Development of the Hydrogeological Model for Investigating the Impact of Contaminant Sources in the Noginsk District, Russia, *Proc. of International Conference on " Groundwater Research - Groundwater'2000"*, Copenhagen, Denmark, 6-8 June 2000, Rotterdam, Balkema, 109-110.
- MCDONALD M., HARBAUGH A., (1988) A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model, *U. S. Geological Survey, Open File Report Washington*, 83-875.
- SLANGENS J., SPALVINS A., (2000) Reliable Program for Preparing Line Data of Hydrogeological Models, *Scientific Proc. of Riga Technical University in series "Computer Science", Boundary Field Problems and Computer Simulation*, Riga, **4**, 42, 41-46.
- SPALVINS A., (2000) Landscape Elevation Map as Reliable Boundary Conditions for Hydrogeological Models, *Scientific Proc. of Riga Technical University in series "Computer Science", Boundary Field Problems and Computer Simulation*, Riga, **4**, 42, 47-50.
- SPALVINS A., JANBICKIS R., (2000) Misfortunes of Zone Scheme Applied for Storing Hydrogeological, *Scientific Proc. of Riga Technical University in series "Computer Science", Boundary Field Problems and Computer Simulation*, Riga, **4**, 42, 28-31.
- SPALVINS A., JANBICKIS R., SLANGENS J., GOSK E., LACE I., VIKSNE Z., ATRUSKIEVICS J., LEVINA N., TOLSTOVIS I., (1996) Hydrogeological Model "Large Riga", Atlas of Maps, *Boundary Field Problems and Computers*, Riga – Copenhagen, 37.
- SPALVINS A., SLANGENS J., (1994) Numerical Interpolation of Geological Environment Data, *Boundary Field Problems and Computers, Proc. of Latvian - Danish Seminar on "Groundwater and Geothermal Energy"*, Riga – Copenhagen, **2**, 35, 181-196.
- SPALVINS A., SLANGENS J., JANBICKIS R., LACE I., GOSK E., (2000a) Methods for Improving Verity of Groundwater Modelling, *Proc. of 16 th IMACS World Congress 2000, Lausanne, Switzerland, 21-25 August*, 6 pages on CDROM, ISBN 3-9522075-1-9.
- SPALVINS A., JANBICKIS R., SLANGENS J., (2000b) Boundary Shells of Hydrogeological Models as Interpolation Devices, *Scient. Proc. of Riga Technical University in series "Computer Science", Boundary Field Problems and Computer Simulation*, Riga, **4**, 42, 32-34.
- SPALVINS A., LACE I., SLANGENS J., JANBICKIS R., (2000c) Improving Verity of Hydrogeological Models due to Heuristic Human Skills Applied within Man-Computer System, *Proc. of the of International Conference on "Simulation, Gaming, Training and Business Process Reengineering in Operations"*, 8-9 September 2000, Riga, 266-270.
- SPALVINS A., SLANGENS J., JANBICKIS R., LACE I., (1999) Reducing of Model Formulation Errors as an Effective Remedy for Improving Simulation Results, *Proc. of International Conference on "Calibration and Reliability in Groundwater Modelling, ModelCARE'99"*, Switzerland, 20-23 September 1999, Zurich, 161-166.
- VAN GENUCHTEN M. Th., (1980) A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils, *Soil Scien. Soc. Amer. Journal*, **44**, 892-898.