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SOFTWARE FOR GROUNDWATER MODELING MAS-2000¹

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Abstract. The article is devoted to modeling of hydrogeological processes by means of package MAS-2000. Development of its basic modules have been done at the end of the last century and now it is adapted for the Windows family operating system. The article contains the brief description of package MAS-2000 and presents its application for numerical modeling of water protection measures for borrow pit (quarry) development.

Key words: ground water modelling, software, mathematical models

1. Introduction

Now mathematical modelling is applied practically in all areas of a science. So for example, on the basis of groundwater modelling (geofiltration and geomigration processes) many applied problems of hydrogeoecology are solved. One of such problems is estimation of influence of groundwater operation on hydrogeological and hydrological conditions of the adjacent territory. As a result of intensive groundwater withdrawal the extensive depression cones are generated in the ground and forcing aquifers, the natural underground flows

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are deformed, the natural watershed are traveled, the level of groundwater is braked from bed of surface current, vertical water interchange between exploitable and overlying aquifers is intensified. This leads to the change of the water balance of the adjacent territory, the groundwater reserve depletion, the reduction of river flows right up to drying up of rivers, the pollution of the exploitable aquifers, and the water quality deterioration on the drinking water supply intakes.

During last years a lot of software implementing different models for modelling the resources and quality of groundwater are developed. Among the software developed in NIS countries we should mention TOPAS (by A.A. Pletnev and L.V. Semendyaeva), MODEL (by I.I. Krashin and E.A. Polshkov) [4] and program package of joint venture *GeoLink* (by A.A. Roshal and others) [3].

TOPAS is oriented for calculation of layers and balances of groundwater in multi-layer aquifers as well as for distribution of concentration and balances of the inert contaminant transferring by the groundwater flow. For solving twodimensional boundary value problems of geofiltration the methods of block relaxation and alternative direction methods with additional modifications for convergence acceleration are used. Calculation of geomigration is fulfilled on the basis of the explicit iterative scheme with discrete correction of the fluxes.

MODEL differs from the previous program by giving users a possibility to take into account capacitive properties of dividing layers and to model the processes of hydrodynamical dispersion, molecular diffusion as well as nonequilibrium sorption which kinetics is given by the linear equation of the first order. For solving boundary value problems of geofiltration and geomigration, the finite difference method is used. Computation of the concentration field caused by the convective transport of contaminants is fulfilled my means of lag calculation. There exists a module for computation the isolines of flow according to the results we get after solving equations of planned geo-filtration in each aquifer. The possibility to work with insets on different scales is implemented.

Program package by joint venture *GeoLink* is designed for modelling and forecasting of processes in subsurface hydrosphere and it includes 15 independent modules. Package for modelling of groundwater filtration allows to compute stationary and non-stationary geofiltration in multi-layer systems and is oriented to solve hydrogeological problems connected with analysis and forecast of groundwater flow. The software for modelling of mass transfer gives a possibility to estimate the change of concentration of chemical component in hydro-geo-chemical system. This change is caused by the convective transport, hydrodynamical dispersion, physical-chemical reactions in the water phase and in the system "water-rock".

The world-wide popular is the software MODFLOW (by Mackdonald and Harbau) [5]. This software is designed for modelling a geofiltration. Boundary value problems are posed in three-dimensions and a wide spectrum of boundary conditions is considered. For solving all mentioned problems different modifications of the finite difference method and method of characteristics are used.

For investigating of migration processes of the contaminants in groundwater a few subpackages of software are developed. They use the original code of data MODFLOW and allows users to carry out computations of convective mass transfer along the lines of flow in MODPATH (Pollak) [9], to take into account anisotropic hydrodynamical dispersion, biochemical reactions of the first order, linear and nonlinear sorption in MODFLOW-SURFACT [7], MT3D96 [8] and others.

The programs using the original code of MODFLOW constitute the basis of GMS (Groundwater Modeling System). GMS works in Windows, has the full colored graphics and a convenient user's interface [6]. The German analogue of GMS is modelling system FEFLOW [2].

For solving specific hydrogeological problems, the proposed software MAS-2000 has no analogue in computational part, but improvement of user's interface is required. The MAS-2000 is used by Belarus scientists for groundwater modelling. Its base modules were developed at the end of the last century [1, 10, 11]. The stages of MAS-2000 development are given in Tab. 1 Now the MAS-2000 is adapted to the Windows operating system.

The developed software provides the receiving of input data on the object under study and hydrogeological parameters of adjacent areas (filtrational properties of porous media, information about external and internal boundary conditions) and visualisation of computational results.

This paper describes the geo-filtration problems solved by using MAS-2000. Effectiveness of using numerical methods for hydrogeological calculations is caused by the possibility of

- development of both regional models of groundwater deposits enclosing large zones and detailed models of specific objects (local model insets) taking into account the complexity of geological, hygrological and hydro-conomic situations;
- solving of inverse (stationary and epignesis) problem of geo-filtration and geo-migration in order to identify the model of the object and natural conditions on the basis of comparison of full-scale and model parameters;
- setting of different boundary conditions including nonstationary ones on the inner and external boundaries of the model.

Numerical modelling provides high accuracy of computations, automation of solution preparation and control of the solution as well as rapid switching to investigation of different variants.

Table 1. The main design determinations of MAS-2000 and their implementation	ation.
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The main design determinations	Multitasking computer-based system for modelling the groundwater flow and evaluation of influence of the water withdrawal on environment									
	Stage I, "Quarry" 1992-1993	Stage II, "Water Scoop" 1994-1995	Stage III, 'SPS-1998 1997-1998	Stage IV, MAS-2000 1998-2001						
Hardware										
Basic PC	AT386	AT486	AT586	PentiumII						
RAM	$4\mathrm{M}$	$4\mathrm{M}$	16M	64M						
Input device of graphical information	digitizer	digitizer	scanner	scanner						
Software										
Operating system	DR DOS 6.0	MS DOS 6.0	Windows 95	Windows 98/NT						
System for graphical information processing	AutoCAD 10	AutoCAD 12	ArcView 3	AutoCAD MAP 4, ArcView GIS 3.1						
Programming system	MS Fortran 5, AutoLISP 10	NDP-Fortran, AutoLISP 11	F32vwb, Avenue	F32vwb, AutoLISP, Avenue						
Informa	ation for hydroe	ecological forec	ast performan	ce						
The model for growndwater flow	single-layer, multi-layer	single-layer, multi-layer	multi-layer, 3D	multi-layer, 3D						
Modelling of geomigration	_	_	convective mass transfer	mass transfer with sorption						
Work with fragments	_	_	+	+						
Determination of geometry of groundwater flows	_	_	_	+						
Determination of water scoop influence zone	_	_	_	+						
Modelling of water-protective measures	+	+	+	+						
Determination of capability of forests and households depend upon groundwate level [2]	- r	+	+	+						

2. Software for Groundwater Modeling MAS-2000

The filtrational problem for multilayered aquifer system is given by the following system of equations:

$$\mu_{i}\frac{\partial H_{i}}{\partial t} = \frac{\partial}{\partial x}\left(T_{i}\frac{\partial H_{i}}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{i}\frac{\partial H_{i}}{\partial y}\right) + G_{r}\left(H_{r} - H_{i}\right) + G_{i-1}\left(H_{i-1} - H_{i}\right) + G_{i}\left(H_{i+1} - H_{i}\right) + Q_{i}, \quad i = \overline{1, n},$$

$$(2.1)$$

where $H_i(x, y, t)$ is groundwater level, $T_i(x, y)$ is aquifer transmissivity, $T_i = k_i m_i$ or $T_i = k_i (m_i - s_i)$, k_i is filtration factor, m_i is aquifer thickness, s_i is groundwater level decline, $G_r = k_r/m_r$, k_r and m_r are filtration factor and thickness of underchannel deposits, correspondingly, H_r is a water level in the river (specified only for the river cells), $G_i(x, y) = k_i^0/m_i^0$, k_i^0 and m_i^0 are filtration factor and thickness of semipermeable separating layers (specified only for the river cells), Q_i is ground water rate, μ_i is specific yield, i is aquifer number, n is total quantity of aquifers. Initial conditions ($H_i = H_i(x, y)$) set distribution of ground waters levels on the territory under investigation during the initial time moment.

Boundary conditions of the first kind $(H_i = \text{const})$ are set if ground water level along boundary is stable (the boundary of intake impact zone, some rivers). Boundary conditions of the second kind $(Q_i = \text{const})$ are set if ground water rate along boundary is stable (some wells and rivers, watersheds, impermeable beds). Nonstationary boundary conditions of the second $(Q_i = Q_i(t))$ are set for ground water intake wells. Boundary conditions of the third kind $(Q_i = Q_i(H_i))$ are set if ground water rate depends on its level (rivers, some kinds of infiltration and evaporation). Boundary conditions of the fourth kind are set on interface of two aquifers and define a continuity of ground water level and flow balance.

The equation system (2.1) already includes the last three boundary conditions. In the case of the stationary filtration regime the right-hand side in equation (2.1) is equal to zero.

To solve the given problem by means of the finite difference method we replace the system of equations (2.1) for each block of the domain under investigation by some finite difference analog. As a result we get a system of algebraic equations, the number of equations is equal to the number of model blocks. For the majority of applied problems the number of model blocks is quite big and it can reach tens of thousands. Physical meaning of the algebraical equations consists in conservation of balance of the fluxes inflowing to the computational block and outflowing from it in the direction of six adjoining blocks having joint edge with the block under consideration.

The time derivatives and the system of algebraic equations are approximated by the implicit difference scheme. For solving the system, the Gauss-Seidel method with relaxation parameter is applied. The result of the solution is the array of groundwater levels for each model block at the given time moment. The division of the filtration domain into blocks is determined by the investigation of the area, density of the located objects, configuration of the hydrographic net, etc. (see Fig. 4).

Since geological medium has laminated structure, the division of the filtration domain into blocks gives us a sequence of horizons in section. These horizons are characterized by the capacity, coefficient of filtration, water yield and porosity. If it is necessary, the horizon could consist of several vertical blocks and be divided into subhorizons. Calculation schemes in section are shown in Fig. 1. The scheme of aquifer draw off, which is realized on numerical model, is shown in Fig. 2.

Thus the computer model of an examined territory takes into account: differences in filtration area structure on the plan and on the section, impermeable beds, site with the absence of aquifers, hydrogeological "windows", rivers and reservoirs with detailed description of the rate and character of the aquifer openings. The following features can be set on the model:

- water intake and injection bore holes with free work condition;
- borrow pits with different variants of their working;
- water economic objects;
- hydrotechnical constructions;
- surface and subsurface reservoirs.

preparation, geofiltration and geomigration calculations.

The MAS-2000 gives a possibility to investigate:

- planned and multilayered geofiltration;
- leakage through semipermeable separating layers and hydrogeological "windows";
- infiltration, evaporation and their change according to the depth of subsurface water level;
- interconnection of surface and ground waters concerning their level separation and close up;
- condition of surface streams and reservoirs (floods, dry weather and drying up of rivers, etc.);
- dynamics of the examined territory hydronet in periods of time.

By means of the MAS-2000 we can solve the following hydrogeoecological problems:

- estimate the ground water resources;
- estimate the anthropogenic activity impact on ground water;
- estimate the groundwater intake influence on natural ecosystems and engineering objects;
- elaborate water-protective measures;
- plan rational water resources development.

Functionally the MAS-2000 consists of four subsystems: input/output data preparation, geofiltration and geomigration calculations.

The initial data of the computer model are the schemes of spatial distribution of hydrogeological parameters on the examined territory.





Figure 1. Calculation schemes in section: (a) zone of hydrogeological "window",(b) zone, where aquifer is absent.

The subsystems of geofiltration and geomigration calculations provides the construction of initial models and the hydrogeological prognosis in the area under study and they are based on the numerical solution of groundwater flow boundary problem.

The general scheme of the MAS-2000, which includes old and new (advanced) modules, is shown in Fig. 3, where the old module (executable file) is called MAS-2000 and new module is called MAS-2000plus. The new executable file for solving geofiltration boundary problem (2.1) by using advanced algorithms, software for visualisation of the input/output information and corresponding examples of numerical models mentioned below are elaborated at financial support of the EC under project INTAS-30-50-4395.



Figure 2. The scheme of aquifer draw off.

The special benchmark task was elaborated for checking operation of new modules. The model itself and boundary conditions are shown in Fig. 4. Variant of display view of this problem is shown in Fig. 5.

During testing of new modules the simulation of ground water intake operating was carried out. Groundwater level decline and water inventory of the area under study are shown in Figs. 6, 7.

For everyone hydrogeological object under study the process of groundwater modeling includes next basic stages (Fig. 8):



Figure 3. General scheme of the MAS-2000 including old and new (advanced) modules.



Figure 4. Calculated model and its boundary conditions (control task).



Figure 5. MAS-2000 display view (control task).

- the correction of the initial model based on solutions of series inverse stationary problems;
- the correction of the model based on solutions of series inverse nonstationary problems (epignosic modelling);
- the prognosis of ground water intake impact, based on a series direct problem solution.

The initial model correction based on a series of inverse stationary problem solution is aimed to receive the computer model, which is adequate to the natural conditions of the examined territory. The criterion of adequacy is the coincidence of model and natural groundwater levels and subsurface flow into the rivers with the given accuracy.



Figure 6. Example of ground water level decline (control task): (a) initial ground-water level distribution, (b) prognosis groundwater level distribution for 180 day.

The initial model correction based on a series back nonstationary problem solution (epignosic modelling) is aimed to receive the computer model, which react adequately on natural and technogenic changes. The criterion of adequacy is the reproduction of the dynamics of ground water levels and subsurface flow into the rivers in natural and changed conditions (the restoration of former condition) with the given accuracy.

In the process of a series inverse stationary and nonstationary problems solution various hydrogeological parameters are specified. The prognosis of ground water intake impact is based on a series direct problem solution and it is aimed on receiving the dynamics of ground water level distribution (or their draw-down), subsurface flow into rivers and water inventory structure

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Aquifer:	1	2	
Inflow through the external bou daries of the 1-st kind, incl.:	^{.in-} 6420.08	5872.23	
western	1631.50	122.07	
eastern	2678.83	461.86 3335.06	
northern	1601.97		
southern	507.78	1953.24	
Inflow through the internal boundaries of the 1-st kind	0	0	
Intake (draw off)	0	-17500.00	
Change of the available supply	y 17.53	2.14	
Recharge, incl.:	13748.87	0	
infiltration	21992.95	0	
evaporatic	on -8244.07	0	
River inflow	-8561.19	0	
Upper inflow	0	11611.87	
Inflow from below	-11611.87	0	
Inflow through the hydrogeological "window"	0	0	
Disbalance m³/day	26.85	-27.53	
%	0.066	0.074	

Figure 7. Example of groundwater inventory (control task)

lritial computer model	back stationary problem solution ⇒	Model, corrected on the results of a series back stationary problem solution	back ronstationa- ry problem solution ➤	Model, connected on the results of a series back nonstationa- ry problem solution	direct problem solution ₽	Prognosis computer model

Figure 8. Basic stages of groundwater modeling.

of the examined territory. The developed numerical model also is used for the construction of filtrational streams in the territory under study.

One of the most important fields of practical application of such numerical models of the saturated flow in porous media is forecasting of ground water quality in the cities when various sources of pollution can take place near groundwater intakes. The information basis of model includes the characteristic of natural (hydrogeological) conditions, and also data on considered anthropogenous loading (existing and perspective). By results of numerical simulation the sources of pollutant which have or can have negative influence on ground water quality are determined. To liquidate the negative influence of anthropogenous loading on quality of drinking ground waters the so-called sanitary protection zone of intake is established [4]. The results of simulation are used by city authorities at the expert estimation of an opportunity of various objects allocation in territory of the sanitary protection zone of ground water intake.

Next important sphere of MAS-2000 application is modeling of the hydrogeological processes, which take place at the development of borrow pit (quarry) of building materials.

3. Model of Borrow Pit

In this year by means of MAS-2000 the borrow pit operating and its impact on adjacent area was carried out. Modeled borrow pit is located in the south of Belarus. The borrow pit development is conducted by open way under water outflow protection. The purpose of researches is to calculate the water protection measures lowering negative influence of the borrow pit on environment.

Preliminary the regional model which is taking into account a long-term plan of borrow pit development for the period of 45 years has been developed. The modeled filtrational area is limited to natural streams and watersheds. In the vicinity of borrow pit the sizes of calculated blocks make 50-100 m, and for peripheries of model increase up to 2 km. In this section the model contains two calculated layers. The top layer consists of the water-sated sand, and bottom represents lean aquifer fissured zone of marl-chalk thickness. For the top layer groundwater flow is free-flow, for bottom layer it is head and free-flow.

The maximal draw-down of groundwater level in borrow pit is 35 m. In result the depression cone size (in isoline 1 m) are 15 km from the east to the west and 14 km from the north to the south. A number of settlements of Byelorussia and Ukraine get to the depression cone of borrow pit. On this territory meliorative systems and wood are located. Wood area is about 27000 hectares and part of its has the reserved status. To decrease borrow pit negative influence on adjoining territory modeling of water protection measures has been executed, it included a hydraulic bar such as recharge channels and forcing wells, antifiltrational bar such as "wall" in the soil (Fig. 9). The water protection measures allow to reduce the depression cone size in 3 times, and on border with Ukraine groundwater drawdown will decrease more than in 10 times and will make less than 1 m.



Figure 9. Scheme of borrow pit development with protection measures lowering its negative influence on environment (compensation activities).

In 2005 the detailed model is developed of borrow pit part, where extraction of sand will be started. The size of calculated blocks make 25 m (Fig. 10).

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Figure 10. Calculated model of the area under study.

As a result of special hydrogeological investigations carried out in the area of open pit, for the numerical model the following parameters were posed (coefficients for the system of equations (2.1)): n = 2, $k_1 = 15$ m/day, $m_1 =$ 16m, $T_1 = 240$ m²/day, $\mu_1 = 0.15$, $k_2 = 5.74$ m/day, $m_2 = 21.6$ m, $T_2 =$ 124m²/day, $\mu_2 = 0.12$, $G_r = 0.13$ day⁻¹, $H_r = 0$, $G_1 = 0.41$ day⁻¹. Ground water rate for the first aquifer is zero ($Q_1 = 0$), ground water rate for the second aquifer consist of two components: rate of intake wells (total value is $Q_2 = (-1920) \div (-2880)$ m³/day, change in time) and rate of forcing wells (total value is $Q_2 = (+960) \div (+1440)$ m³/day, change in time).

We specify the following initial conditions: $H_1(x, y, 0) = 0$, $H_2(x, y, 0) = 0$ and boundary conditions: $H_1(x, y, t) = 0$, $H_2(x, y, t) = 0$, $(x, y) \in \Gamma$.

Simulation results show that exploiting of the pit could decrease the groundwater level on the boundary between Belarus and Ukraine for more that 1 m. This could bring to the disturbance of the water regime of soil and degradation of the growth (see Fig. 11). Therefore compensation activities are necessary. Two variants of compensation activities were elaborated for localization of depression cone:

a) to use the recharge channels (variant 1),

b) to use the forcing wells (variant 2).

After compensation activities the groundwater drawdown on the border is less than 1 m (see Fig. 12). For modeling the influence of forcing wells the special software has been developed. It allow to automate selection rating of well and to provide localization depression cone in the chosen directions. A.Smychnik et al.



Figure 11. Forecast of decline of groundwater level: (a) view in plan, (b) 3D-view.



Figure 12. Forecast of decline of groundwater level with compensation activities (fragment of calculation model): (a) variant 1 (recharge channels), (b) variant 2 (forcing wells), (c) 3D-view.

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