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Modelling of groundwater flow dynamics and contaminant transport processes for the Bernau area, Germany

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ABSTRACT: The Bernau place in Germany is heavily polluted with tetrachlorethane. To help in solving the remedy problem of the place, a system of hydrogeological models (HM) has been developed by the Environment Modelling Centre (EMC) of the Riga Technical University.

1 INTRODUCTION

During 1935-1990, the Bernau place (located ~50 km north of Berlin, Germany) has been polluted with tetrachlorethane (TCE), which is the DNAPL (dense non aqueous phase liquid) type substance. It sinks in groundwater until the nearest aquitard is reached. Due to this feature, the lateral motion of TCE is controlled both by the hydraulic gradient of groundwater and by the slopeward top surface of the aquitard. If the surface includes some pit, TCE may accumulate here. In 2001, the German hydrogeological company INGAAS GmbH has started a cleaning plant (CP) for in-situ remediation of contaminant groundwater in high concentrations (75-300 mg/l). The construction of CP consists a groundwater accumulator, which feeds the reactor where dehalogeniation of TCE is accomplished. The accumulator occupies the centre of the TCE spill, which is framed by a vertical impermeable wall. Contaminated groundwater is injected at the bottom part of the accumulator, and its groundwater table uplifts. Due to an additional hydraulic gradient, groundwater passes through the reactor. Cleaned water is infiltrated into the ground. It is expected that the contaminated soil, within the accumulator, will got gradually cleansed because of TCE - wash out there.

Although general ideas of how CP should be built and controlled afterwards are clear enough, there is a lot of questions to be answered if practical details are considered:

- How does the system "accumulator → reactor" work? What factors do control its productivity?
- How will CP interact with the environment? What is the best choice of the groundwater pump-out and reinfiltration places and regimes?
- How does TCE spread out regionally? What are the optimal measures to stop this processes?

To answer these questions, rather ample modelling has been accomplished. Its main results are discussed in this paper, which is based mostly on materials of the contract reports of EMC (Report 1999, Report 2001a, Report 2001b, Report 2001c, Report 2001d). All information used for creating and calibrating of Bernau HM was provided by INGAAS GmbH.

2 SUMMARY ON MATHEMATICS AND MODELLING METHODOLOGY APPLIED

Regional and local HM were created to investigate the Bernau case. Their layout is shown on Fig. 1. Regional and local HM cover 1.2 km $*$ 0.8 km = 0.96 km^2 and 0.23 km $*$ 0.17 km = 0.039 km^2 areas, correspondingly.

To elucidate the main problems associated with creation of HM, it is necessary to discuss some mathematical procedures applied. According to the semi-3D approximation scheme, the *xyz*-grid of HM is built of ($h * h * m$)-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 the number of aquifers and interjacent aquitards, accordingly. Its four vertical sides compose the shell of the HM grid. For regional and local Bernau HM , h=10 and 2 meters, respectively; $s = 9$ (see model schematization in Fig.1).

The relief (ground surface *relh*) and the lower side of the model are its geometrical top and bottom, respectively. The vertical size of Bernau HM does not exceed 45 meters. The 3D-space volume enveloped by the boundary surfaces constitutes the body of HM.

The vector φ 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:

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

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 ψ are specified; in Bernau HM, the ψ-distribution exists on the whole HM surface, and the source vector β contains only rates of the groundwater withdrawal or infiltration in wells; β_ψ is the computed flow passing through elements of the diagonal matrix G. . In Bernau HM, the ground surface map ψ_{relh} and $\psi_{L5} = 60$ m asl are used as boundary conditions

Each grid xy-plane contains $n_{xy} = n_x * n_y$ nodes (n_x and n_y represent, accordingly, the number of nodes on the x and y sides of the plane). The grid of (1) contains $N = n_{xy} * (s+1)$ nodes. For regional and local Bernau HM, n = 121 $*$ 81 $*$ 10 = 98,010 and 116 $*$ 86 $*$ 10 = 98,600 nodes correspondingly. The elements a_{xy}, a_z of symmetric A_{xy}, A_z (or g_{xy}, g_z as constituents of G) are computed, as follows:

$$a_{xy} = k\,m, \quad a_z = h^2 k / m, \quad k \geq 0, \quad m_i = z_{i-1} - z_i \geq 0, \quad i = 1,2,...,10 \tag{2}$$

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 ψ_{rel} with the hydrographical network included; m, k are, accordingly, elements of digital m, k–maps of the computed thickness and permeability of layers. Permeability values of aquifers and aquitards differ drastically: they are (1 - 50) and (10^{-2} - 10^{-6}) meters/day, respectively.

The set of the z-maps describes the full geometry of HM. Usually, 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. Bernau HM includes three discontinuous layers (*aS2, LS2, bS2*).

In modern modelling systems, the m-maps are never computed directly from data of geological thicknesses applied as initial data, because this approach may result in serious errors of the HM geometry.

The following software tools were used for creating Bernau HM:

- the REMO system for creating and running HM (Spalvins et al. 1996);
- the GDI program (Spalvins and Slangens 1994) for building digital k, m - maps of (2);
- the Groundwater Vistas (GV) system (Environmental Simulation 1997) for implementing contaminant mass transport model (TM) on the MT3D'99 code (Papadopulos 1999);
- the SURFER program (Golden Software 1997) supports graphics, digitises electronic images and performs grid mathematics.

Hence the REMO system prepares HM as the driver for TM, REMO is compatible with the MODFLOW system running HM (McDonald & Harbaugh 1988), in the GV environment.

In REMO, solution of (1) is obtained, as the following superposition:

$$\varphi = \varphi_S - S \,, \tag{3}$$

where φ_S is the conditionally "undisturbed" solution if $\beta = 0$ (no pumping wells are active); S is the drawdown distribution when $\beta \neq 0$, $\psi = 0$. The superposition (3) is handy for the Bernau case when boundary conditions on the shell surface of local HM should be obtained as a part of the corresponding regional solutions for the φ_S, S distributions.

In Bernau HM, results of pumping tests were used for calibration of the k – maps. In a grid of HM, the following problem should be overcome, to accomplish such a calibration correctly:

- water extraction wells are located irregularly with respect to nodes of an HM grid; in REMO, to improve accuracy of modelling, a pumping rate of a well is interpolated to the four nearest nodes (in MODFLOW, the rate is roughly moved into the one nearest node);

- the interpolated rates produce the depression cone with the smaller depth than the single noninterpolated rate does, when located exactly in the node;
- to account for this feature of the interpolated rates, the "true" value of the depression cone depth must be computed by the special back – interpolation program of REMO (Spalvins et al. 1995);
- no grid can directly provide the right value of the drawdown S measured in a well of a diameter d_w under pumping conditions, because each node of the grid acts like a well with the equivalent diameter $\sim 0.4\ h > d_w$; for this reason, the grid provides the drawdown $S_{gr} < S$. The necessary value S is obtained by the following analytic correction:

$$S = S_{gr} * c_{gr}\,, \qquad c_{gr} = 1 + \ln\,(0.4\ h\,/\,d_w\,)\,/\,\ln\,(D_{\mathrm{w}}\,/\,0.4\ d_w) \tag{4}$$

For Bernau HM, D_{w} = 500 metres is applied. It follows from the above explanation that one should be careful to apply results of pumping tests for calibration purposes, because two independent factors (interpolation, an analytic correction) should be correctly accounted for.

3 MODEL GEOMETRY

In Bernau, two sandy Quaternary aquifers *L2* and *L3* are TCE – contaminated, and they are represented in the model schematization (Fig. 1). To obtain the *z* – maps for the regional HM, an enlarged 1.4 km $*$ 1.8 km model area was used (Report 2001a). The area included ten deep wells, as sources for geometrical data. Regional HM occupies only a central part of the enlarged area.

In HM, the unsaturated part of the *L2* aquifer – the aeration zone *aer* is treated like an aquitard. The saturated part of *L2* is represented by four subaquifers *L2a, L2b, L2c, L2d* of equal thicknesses. The vertical transmissivity of *L2* is accounted for by introducing three formal subaquitards *i2a, i2b, i2c.*

The aquitard *S2* contains the fine sand lens *LS2.* For this reason, two subaquitards *aS2, bS2* are applied. The *S2* aquitard contains a large hydrogeological window (Fig.1). However, its real geometry is unknown. For this reason, its influence is accounted for by controlling the *k*-maps here.

The *L3* aquifer is composed of three sublayers *L3a, L3b, L3c* joined by two formal aquitards *i3a, i3b*. The sublayers *L3b* and *L3c* have equal thicknesses. The thickness of the *S4* aquitard is conditionally assumed to equal 5 meters. The mean thickness of the Teufel pool was assumed to be ~2 meters, and the pool is sited in the *L2a* aquifer.

For Bernau HM, the fine geometrical schematization is applied, because of the following reasons:

- both *L2* and *L3* aquifers are heterogeneous if their permeability is considered;
- the wells tried for pumping tests have different lengths of screens; for short screens, depression cones in neighbouring subaquifers differ considerably;
- it is possible to place contaminant sources, applied by the MT3D code, in different positions within the *L2* and *L3* aquifers;
- in local HM, one can simulate the system "accumulator – reactor" with a good accuracy.

The real thicknesses m_{aer} of the *aer* zone was computed when the calibrated φ - distribution was obtained:

$m_{aer} = \psi_{rel} - \varphi_{L2a}$ if infiltration was positive (recharge),
$m_{aer} = 0.02$ metres if infiltration was negative (discharge).

Until HM was not calibrated, the initial thickness $m^o_{aer} = 0.02$ metres, everywhere (Spalvins 2000).

The of top surfaces the *S2* and *S4* aquitards descend in the southern direction, and the TCE – migration there may follow this route.

The geometry of local HM is built by using data provided by the regional *m*–maps.

4 PERMEABILITY MAPS

Satisfactory initial data for permeabilities of aquifers were available only for the area of local HM. They enabled to obtain the *k*–maps of good quality there. Considerable part of initial data were specified by simulating pumping tests for the wells. It follows from (Report 2001d) that the permeability of the *L2* and *L3* subaquifers is very heterogeneous. The permeability values vary from 10 - 49 m/day and 1.9 – 28.0 m/day for the

L2 and *L3* aquifers respectively. The *k*–maps of the *L3b* and *L3c* subaquifers were identical, but the *L2a, L2b, L2c, L2d, L3a* layers had different maps. For the aquitards *S2* and *S4*, $k = 0.86 * 10^{-2}$ m/day and $0.5 * 10^{-4}$ m/day was applied, accordingly. In the *S2* window, $k = 0.43 * 10^{-1}$ m/day and 15 m/day were used, correspondingly, for the *aS2* and *bS2* aquitards.

In Bernau HM, the following formula was used for the vertical transmissivities a_z of the formal subaquitards in the *L2* and *L3* aquifers:

$$a_z = h^2 k_f \ c_a / m_f \tag{5}$$

where c_a, k_f, m_f were the anisotropy factor, the permeability, the thickness, respectively, of the aquifer sited above the subaquitard considered. For the *L2* and *L3* aquifers, $c_a = 0.25$ and 0.1 were used, correspondingly.

5 BOUNDARY CONDITIONS

On the regional HM shell (four vertical sides of HM), the initial data for boundary conditions were taken mostly from the maps where locations of the piezometric head isolines were shown. The infiltration flow on the HM top was governed by the ground surface map ψ_{relh}. This map also helped to fix the boundary conditions for the shell of the *L2* aquifer. For the *L3* aquifer, an almost linear distribution of the boundary head, on the northern and southern sides of HM, was applied.

It follows from Fig. 1 that groundwater flow, in the *L2* aquifer, is more intensive for the eastern part of HM. The Teufel pool collects nearly all groundwater flow coming from this part. The isoline pattern in the western part of the *L2* aquifer is distorted both by the Teufel pool and the hydrogeological window of the *S2* aquitard (Report 2001b). The groundwater flow is very slow there.

In the *L3* aquifer, the groundwater flow is much slower than in the *L2* aquifer (see vertical section of Fig.4). Under influence of the *S2* window and the Teufel pool, the groundwater flow of the *L3* aquifer declines in the SW direction, from the expected WE line controlled by the boundary conditions on the *L3* shell.

For local HM, boundary conditions on its shell are taken from the corresponding regional distributions of φ_S and *S* for the superposition (3).

6 RESULTS PROVIDED BY HYDROGEOLOGICAL AND TRANSPORT MODELS

For the TCE – contaminated Bernau area, regional and local HM have been created. They have been used as drivers for TM applied for investigating contaminant transport processes at regional and local scales. The following main results have been obtained:

- the Teufel pool is the main element controlling regional migration of contaminants; detailed numerical experiments regarding the water balance of the pool have been accomplished; it have been found out that, probably, only a small part of TCE enters the pool, because TCE migrates mainly above the top surface of the S2 aquitard there; until now, this guess is not confirmed experimentally, because at vicinity of the pool no monitoring wells are available yet;
- detailed calculations of the water balance have been done for regional HM and for its main elements (Report, 2001c); these results enable to estimate the influence of any element (pools, ditches, borderlines, etc.) on the 3D – distribution of the groundwater flows in aquifers and aquitards; for example, the northern ditch may considerably redistribute the flow in the *L2* aquifer; the ditch may also catch a considerable part of TCE; unfortunately, no data about the construction of the ditch is available (open row or buried drain?); during summertime its impact is negligible and most of the TM experiments have been performed when the influence of the ditch was not accounted for;
- an impact of the former waterworks on the TCE – migration has been evaluated; it follows from MT3D results shown in Fig. 2 that two production wells TBr1, TBr2 withdrawing water from the *L3* aquifer drastically alter the transport of TCE – if these wells are operational, they pump out practically all TCE; as it follows from graphs of Fig. 3, this process starts after ~400 days; without waterworks, some loss of the TCE mass begins after ~4,000 days when the spill plume reaches the Teufel pool and then no less than ~2,000kg of TCE are resident in groundwater;

- modeling confirmed that contaminated groundwater can be withdrawn effectively from the *L2* and *L3* aquifers if the screens of the pumping wells are sited in *L2d* and *L3c* subaquifers, respectively, if the supply of the CP accumulator is considered;
- there is a problem of reinfiltration of cleaned water into the ground; if this operation is accomplished uncorrectly then some unwanted increase of the TCE contaminated area may occur, and the productivity of CP may worsen (Report 2001b);
- the impermeable walls of CP considerably disturb the groundwater regime there (see Fig. 4); it should be accounted for when some further research, regarding regimes of CP, will be performed.

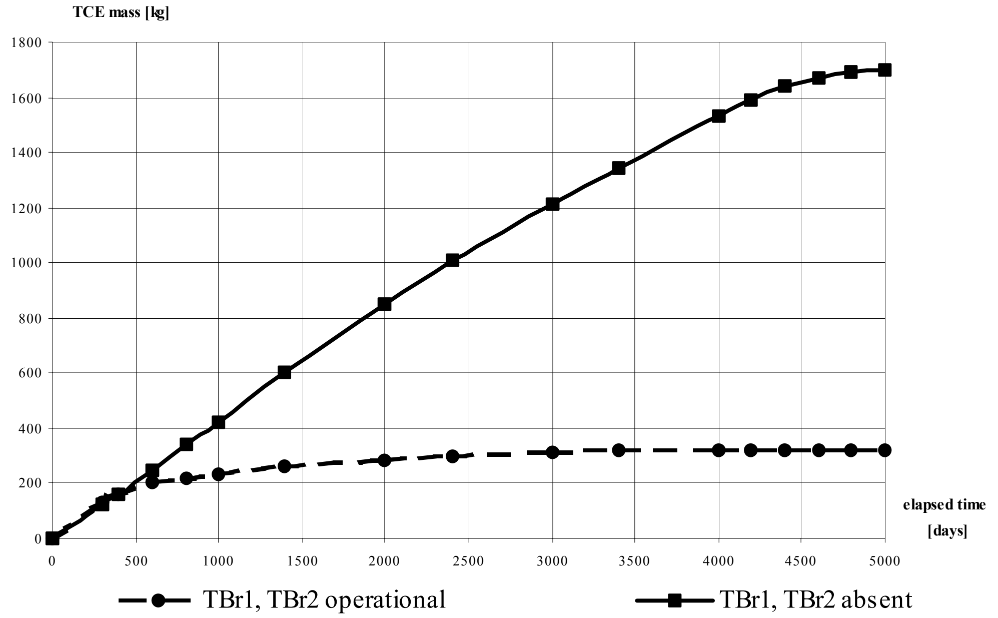

Fig. 3. The MT3D – computed graphs of the TCE mass

7 CONCLUSIONS AND RECOMMENDATIONS

Considerable research has been accomplished to create mathematical models for investing the problem of remediation for the TCE – contaminated Bernau area. The local HM is ready for necessary investigations regarding performance of the cleaning plant.

However, initial data used for creating of the models were rather scarce. Presently, all models are open for necessary further corrections and improvements, when new field data will be available.

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Обьект Бернау в Германии сильно загрязнен тетрахлоретаном. Центр Моделирования Окружающей Среды, Рижский Технический университет разработал систему гидрогеологических моделей, помогающих решить проблему очистки этой местности.