Modelling of groundwater flow dynamics and contamination transport processes at the Vilnius oil storage area

AIVARS SPALVINS, ROMANS JANBICKIS, JANIS SLANGENS, INTA LACE
Environment Modelling Centre, Riga Technical University, 1 Meza Str., LV 1048 Riga, Latvia
e-mail: emc@egle.cs.rtu.lv

ANTANAS MARCIONIS & ANICETAS STUOPIS
Hydrogeological Company GROTA, 26 Eisiskio Plentas, LT 2038 Vilnius, Lithuania

Abstract The Vilnius oil storage area is polluted with light oil products migrating in groundwater towards the Neris River and two nearby well fields. Hydrogeological and transport models were developed to investigate this migration. Advantages and drawbacks of the software used are described and modelling results reported.

HYDROGEOLOGICAL MODEL

In the Vilnius oil storage area (OS), the 30–50 cm thick, free oil body slowly floats in groundwater, and the rather fast moving dissolved oil fraction (~15 mg l^{-1} in OS) may reach the Neris River (Fig. 1). Chloride tracing (UAB GROTA, 1997) indicates that, via hydrogeological windows, dissolved oil may descend into the productive aquifer which supports two well fields (Railway Co., Vingis). The protective horizontal drain (Fig. 1) was installed to collect contaminated groundwater (~1000 m^3 day^{-1}). However no proof existed that the drain would stop the dissolved oil movement towards the well fields. The Environment Modelling Centre (EMC) of the Riga Technical University and GROTA, Vilnius, created hydrogeological and transport models (HM and TM) of the OS area to enable investigation of this. The results, discussed in this paper, are mostly based on a report (Riga Technical University, 1998).

Modelling of dissolved oil migration was performed only for the HM centre—within the 1.5 × 2.0 km area (Fig. 1). It is surrounded by a buffer zone which enables the depression cones of both well fields to be accounted for.

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 s-tiered xy-layer system (s is the number of strata involved). Its four vertical sides compose the shell. In the OS case, h = 50 m, and s = 11 (six aquifers and five intervening aquitards are accounted for).

The quasi-three-dimensional (3-D) steady state HM was applied to compute the mean annual piezometric head distribution φ, in nodes of the HM grid, as the numerical solution of the following algebraic equation system:

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

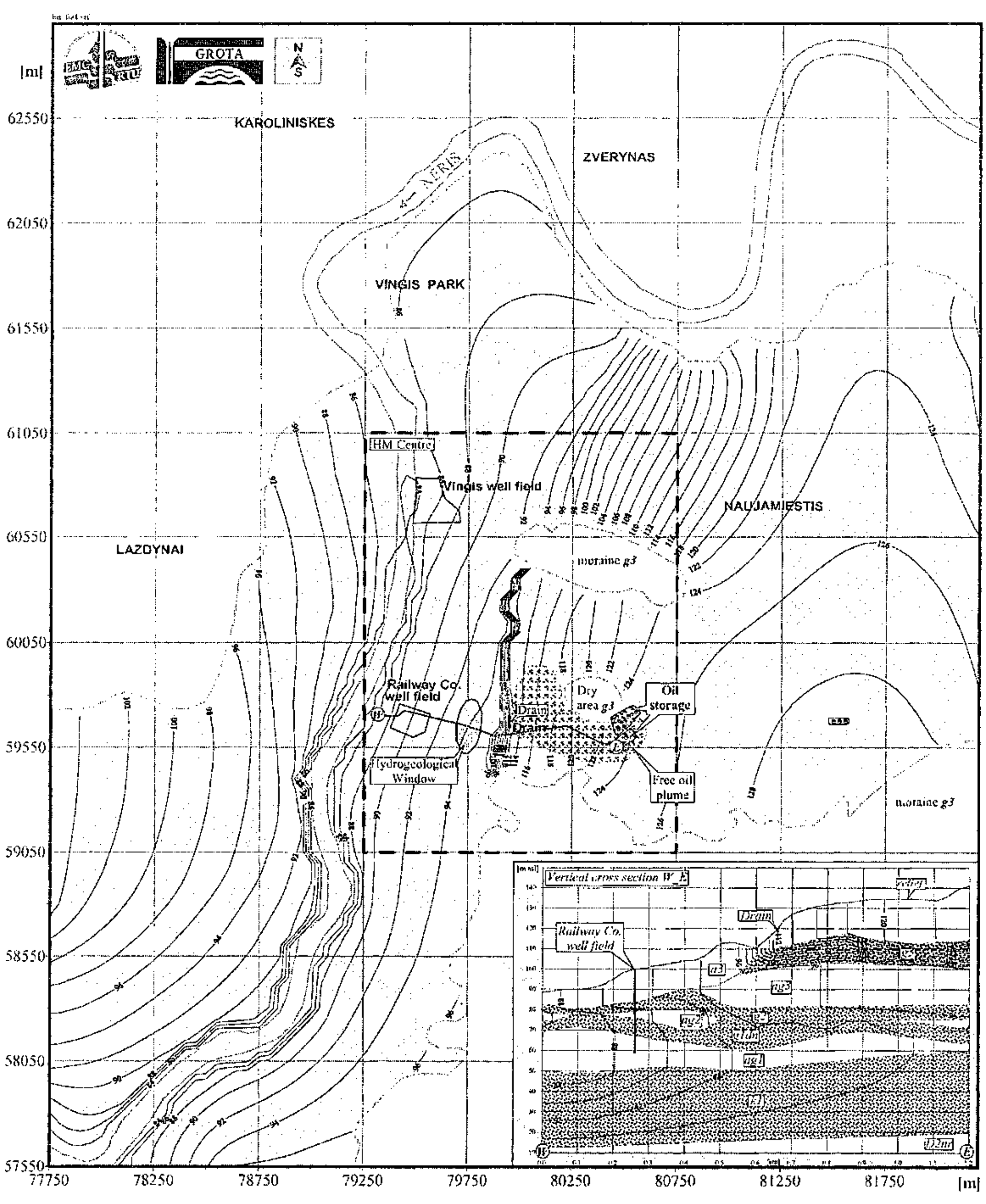

Fig. 1 The piezometric head distribution (m a.s.l.) of aquifer **a3** assuming the Vingis and Railway Co. well fields have water intakes of 8300 $m^3 day^{-1}$ and 1200 $m^3 day^{-1}$ respectively. The vertical cross section WE is shown.

where the matrices A_{xy}, A_z, G, represent respectively, horizontal links of aquifers (arranged in six xy-planes), vertical links (originating in the five aquitards) between the adjoining xy-planes, and elements connecting nodes of the grid with the piezometric boundary conditions ψ; the vector β accounts for boundary flows.

The elements a_{xy}, a_z of the matrices A_{xy}, A_z, are computed by using digital maps of the thicknesses m, m_0 (heights h_z) and permeabilities k, k_0 of the aquifers and aquitards. The following formulae are applied:

$$a_{xy} = k\,m, \quad a_z = h^2 k_0/m_0, \quad k, k_0 \geq 0, \quad m, m_0 = H_{i-1} - H_i \geq 0, \quad i = 1,2,\ldots,11 \qquad (2)$$

where H_{i-1} and H_i are the top and bottom surfaces of the ith stratum, respectively; H_0 represents the relief with the hydrographical set included.

Each of six xy-grid planes extends over the 4.25×5.45 km area (Fig. 1) and contains $90 \times 110 = 9900$ nodes. The whole grid has $6 \times 9900 = 59\,400$ nodes. Accordingly, the planes 1,...,6 represent: the map of the relief **relh** elevations, four Quaternary aquifers **a3**, **ag3**, **ag2**, **ag1**, and the Devonian aquifer **D2nr** head distribution. The planes 1 and 6 carry boundary conditions ψ, on the top and bottom surfaces of HM, respectively. The conditions ψ are also fixed on the shell of HM and on the drain, in the aquifer **a3.**

The vertical links a_z are originated by five aquitards: **aer**, **g3**, **g2**, **g1dn**, **k1**. The aquitard **aer** is formal and gives the vertical grid conductivity of the unsaturated aeration zone. The infiltration rate here is the flow between the **relh** and the first unconfined aquifer underneath.

All strata, but **ag1** and **k1**, include areas with a zero thickness $m,m_0 = 0$ (the shape of the discontinuous aquifer **a3** is shown in Fig. 1). For this reason, the H-surfaces of equation (2) were created using the Geological Data Interpolation (GDI) program (Spalvins & Slangens, 1994), because it always holds the condition $m,m_0 \geq 0$ of equation (2) and acquire $m,m_0 = 0$, where necessary. Since the GDI program can use lines as information carriers, a rich set of the available geological cross sections was applied as initial data for generating the H-surfaces. The k,k_0-distributions of equation (2) were also obtained using this program.

Due to the presence of numerous $m,m_0 = 0$ areas, the groundwater flow dynamics of the OS area are complicated, and the calibration of HM was not easy. We will only outline the most important facts accounted for by HM:

- in the oil contaminated aquifer **a3** downgradient from OS, on the abrupt edge of the moraine **g3**, an underground "waterfall" occurs because the head difference over a short distance is nearly 15 m (Fig. 1);
- in the zone of the waterfall, the aquifers **a3** and **ag3** are directly connected;
- in aquifer **a3**, northward of OS, the dry area is formed by the uplift of the moraine **g3**; the size of the area depends on the saturated thickness of **a3** here;
- the hydrogeological window (in aquitards **g2** and **g1dn**, the permeability k_0 is increased here) allows dissolved oil to descend from aquifer **a3** into the productive aquifer **ag1**.

The REMO code was applied for developing HM, because of the following advantages (Spalvins *et al.*, 1995; Spalvins *et al.*, 1999):

- the impact of human errors is greatly reduced, because all maps of HM can be obtained from the initial data by the GDI program which is in a perfect synchronism with REMO;
- the map of landscape relief elevations is used for controlling the infiltration flow. Four variants of HM were created, to account for the influence of the drain

(normal, lengthened, no drain), and the impact of intake rates (normal, maximal) at the well fields.

The Groundwater Vistas (GV) code (Environmental Simulations, 1997) was used to join HM and TM. REMO data files were exported in GV. Unfortunately, the HM data needed revision afterwards, because they were distorted by GV during this exportation. This annoying side effect of GV is caused by the memory saving zone principle used by this code (Spalvins *et al.*, 1999).

MASS TRANSPORT MODELLING

The main results from TM of OS were obtained by applying the MT3D'96 code. Later, some experiments were accomplished using the newest—MT3D'99 version. Both codes are installed in GV.

Generally, TM is driven by HM, and TM is controlled by the following main transportation parameters (Papadopulos, 1996, 1999):

- the spatial distribution of contamination sources and their concentrations;
- the regime of contaminant particle tracking (advection only, cf. sorption and destruction accounted for); two parameters are available to set the regime: the sorption coefficient k_d and the half-life time $t_{0.5}$ of the contaminant ($k_d = 0.5$, $t_{0.5} = 500$ days, were tried to account for sorption and destruction, respectively);
- the method of contaminant particle tracking (four methods are available, but the method of characteristics (MOC) was used for the OS case); each method should be adjusted by applying its specific control parameters;
- the choice of the simulation time step Δt; regimes for saving results and printout (Δt = 20 days and 2 days were used by MT3D'96 and MT3D'99 codes, respectively).

The area, in the aquifer **a3**, where the free oil plume has been observed coincides with the set of TM contaminant sources (about 70 cells if a grid block has one cell). However, this full set was not used in TM, because of the following reasons:

- no reliable data were available regarding the dissolved oil concentration distribution within the plume area;
- the full set did not allow investigation of contamination dynamics at specific important spots of OS;
- under the complex hydrogeological conditions of OS, the autostop of the MOC method happened very rapidly if all 70 cells were used.

For these reasons, four small concentration sources with the constant relative concentration $c = 100\%$, were used. Each was chosen to investigate a different problem. For example the first source (four cells) showed how oil migrated from the OS centre towards the drain and tested the influence of the drain. The fourth source (two cells) was located in the centre of the hydrogeological window (Fig. 1); it was expected that it should help understanding of the role of this window in possible contamination of the well fields. Even using these simple sources, experiments with the MT3D'96 program demonstrated the following unpleasant side-effects:

- no long term predictions (more than 500–1000 days) can be obtained for the OS case, because computations are soon stopped automatically;

- even before the termination, obvious indications of computational instability can be observed: isolated non-zero concentration spots far from the main concentration areas, chaotic concentration changes in monitoring wells, an incorrect total contaminant mass balance, etc.

We suspected that the above drawbacks were due to both the complexity of HM and the MT3D'96 code's inability to cope with it. Later, some key experiments were repeated by using the recent MT3D'99 version. The results obtained fully confirmed our suspicions: no auto-termination of computations occured, even if, instead of the time step $\Delta t = 20$ days (used by MT3D'96), $\Delta t = 2$ days was applied; the computational instability indications also diminished considerably.

However, in spite of the difficulties caused by the MT3D'96 code, about 50 experiments (variable: HM, concentration sources, regimes of particle tracking) were performed, and quite reasonable results were obtained (Riga Technical University, 1998), and were used by the GROTA company, Vilnius.

CONCLUSIONS

Modelling of dissolved oil migration, in the area of the Vilnius oil storage, has been performed, in the Groundwater Vistas environment, by using the MT3D'96 and MT3D'99 codes. The recent MT3D'99 version proved to be considerably stronger than the MT3D'96 code. The modelling provided the following main results:

- the horizontal drain gives considerable protection against the mobile oil migration; however, it cannot completely prevent the movement of dissolved oil towards the Neris River and through the hydrogeological window, in the direction of the Railway Co. well field;
- sorption and destruction processes may considerably slow down the dissolved oil migration; however, more exact data regarding these processes are needed to make realistic prognoses;
- to solve the problem of optimizating protective drain construction, a more detailed model should be used for this area; its plane approximation step must not exceed 5–8 m.

REFERENCES

Environmental Simulations, Inc. (1997) *Groundwater Vistas*. User Guide. Environmental Simulations, Inc, 2997 Emerald Chase Drive, Suite 100, Herndon, Virginia 20171, USA.

Papadopulos, S. & Associates, Inc. (1999) *MT3D'99*. User's Guide. Environmental and Water-Resource Consultants, 7944 Wisconsin Avenue, Bethesda, Maryland 20814, USA.

Papadopulos, S. & Associates, Inc. (1996) *MT3D'96*. Documentation and Input Instructions. Environmental and Water-Resource Consultants, 7944 Wisconsin Avenue, Bethesda, Maryland 20814, USA.

Riga Technical University (1998) Modelling of Groundwater Flow Dynamics and Contamination Transport Processes at Area of Vilnius Oil Storage. Contract No.6274/98 Report, Riga, Latvia.

Spalvins, A. & Slangens, J. (1994) Numerical interpolation of geological environment data. In: *Proc. Latvian-Danish Seminar on Groundwater and Geothermal Energy* (Riga-Copenhagen), vol. 2, 181–196. (*Boundary Field Problems and Computers* 35).

Spalvins, A., Janbickis, R., Slangens, J., Gosk, E., Lace, I., Viksne, Z., Atruskievics, J., Levina, N. & Tolstovs, J. (1995) Development of regional hydrogeological model "Large Riga". In: *Proc. Int. Seminar on Environmental Modelling* (Riga-Copenhagen), vol. 1, 145–158. (*Boundary Field Problems and Computers* 36).

Spalvins, A., Slangens, J., Janbickis, R. & Lace, I. (1999) Reduction of model formulation errors as an effective remedy for improving simulation results. In: *Calibration and Reliability in Groundwater Modelling* (Pre-published Proc. ModelCARE'99 Int. Conf., Zurich), 161–166.

UAB GROTA (1997) In: *General Information, NATO Advanced Research Workshop on Environmental Contamination and Remediation Practices at Former and Present Military Bases*, Vilnius, 16–20.