Pollution of underground water—a computational case study using a transport model

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ABSTRACT

Damage of the waterproofing system in a waste material depository or sewage sludge composting plant and the penetration of pollutants into the soil and groundwater may cause an environmental mishap. Although the standard waterproofing technologies are extremely safe, one cannot disregard possible malfunctions. For a well-established plan of managing unexpected events, the impact of such damage must be forecast. With the help of models described in the relevant literature, we propose the basic ideas used in simulations for two planned regional waste material depositories, a planned sewage sludge composting plant and an active aluminium dross depository of a foundry.

Key words | underground water, pollution, transport model, case study

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INTRODUCTION

When building a waste material depository or sewage sludge composting plant, damage of the waterproofing system is regarded as a possible malfunction. The penetration of pollutants into the soil and groundwater causes environmental damage. Since the standard waterproofing technologies are extremely safe, the probability of environmental pollution caused by the failure of waterproofing is very small, but it cannot be excluded. Hence, in addition to the effort in the interests of maximum safety, the elaboration of a plan for managing unexpected malfunctions and possible damage becomes a fundamental requirement. As usual, state laws impact on this requirement, too.

In order to trace the spread of pollutants in the groundwater after a mishap, the concentration of groundwater pollution in the damageable area can be well estimated by the use of models described in the relevant literature. In this paper, we describe the basic ideas used in calculations. They concern two planned regional waste material depositories to be built in the vicinity of the Hungarian villages Gyál and Taksony, a planned sewage sludge composting plant near the town of Dunaharaszti and an active aluminium dross depository at a foundry near the village of Apc. These predictions resulted in a relatively low level of pollution. They formed part of the analysis in the environmental impact assessments submitted for gaining permission from the authorities for environmental protection. The other parts of the analysis made in cooperation with other institutions and firms will not be discussed here.

It is well known that groundwater pollutants may involve severe consequences when live water, wells and water bases are affected. The laws of the spread of pollutants in groundwater can be described approximately by transport equations. Their solutions describe the concentration of pollutants. Knowledge of the concentration level is a prerequisite for finding efficient ways for both the prevention of further spread and the removal of pollutants from the groundwater.

The transport equations contain various parameters. Their identification can be difficult and their values may still remain inexact. Our experience was, however, that in the actual parameter range we get satisfactorily correct results, suitable for evaluating the environmental situation.

Different forms of the transport equation that are valid locally are well described in the literature and are explained even at the textbook level (see, e.g., Kovács &

Table 1 | Physical parameters

Parameter	Meaning	Minimum value	Typical value	Maximum value	Dimensions
v_x	Infiltration speed	0.75	1.5	3	m/d
R	Delay factor	1	1.2	1.5	—
α_L	Longitudinal dispersity	20	25	31.5	m
λ	Decay rate	0	0	0.0001	1/d
n_0	Porosity	0.12	0.15	0.18	—

Szabó 1995). Depending on the complexity of the global model, its solution is obtained either by closed formula or, more frequently, by numerical methods. For the first case, one can be advised by texts on mathematical physics (see, e.g., Tikhonov & Samarskii 1966) or, alternatively, numerical methods must be involved. Detailed studies cannot be managed without computer support.

For the first evaluation of a mishap, a simple model borrowed from Kovács & Szabó (1995) and modified slightly turned out to be satisfactory. In the next section, we describe the transport model applied to the phenomenon under consideration.

THE TRANSPORT MODEL AND ITS COMPUTATION

For the first approximation of the transport process, several assumptions can be made. In the coordinate system with coordinates x, y, z, the ground surface is approximated by the coordinate plane (x, y). The boundary of the impermeable layer is parallel to the ground surface and is located at depth $z=m$. The cylindrical waste depository with its axis along the z axis is assumed to have a negligibly small cross section with respect to the size of the domain where the pollution permeates. Thus, a line source between the two planes along the z axis acting over the period $0<t<T$ is considered. The infiltration has a prevailing direction. The x axis is chosen in this direction and the y axis is perpendicular to it. In the prevailing direction x, the infiltration has a constant speed v_x in the whole region. In directions different from x, the infiltration is neglected. As is widely used in the literature, in the unbounded three-dimensional domain $-\infty<x,\ y<\infty,\ 0<z<m$, we model the convective–dispersive transport phenomenon by a quasi-linear parabolic equation for $t>0$:

$$Rn_0c_t + v_xc_x = \alpha_Lv_xc_{xx} + \alpha_Tv_xc_{yy} + \alpha_Tv_xc_{zz} - \lambda Rn_0c + f(x,y,z,t). \quad (1)$$

In this equation, $c(x,y,z,t)$ (in brief, c) stands for the unknown concentration and the subscripts t, xx, yy and zz refer to the first and second partial derivatives with respect to the indicated variables. The meaning of the physical parameters R, n_0, α_L and λ, together with their most frequent values, as well as for v_x is extracted from Kovács & Szabó (1995) and given in Table 1. Comments on the transversal dispersity α_T will follow in the next section.

The depository located at the origin begins leaking at $t=0$. The intensity of leaking is time-independent until stopped at $t=T$ and it varies smoothly with respect to the depth z. Thus, the line source used in the model is

$$f(x,y,z,t) = \delta(x)\delta(y)q(z)(\theta(t) - \theta(t-T))$$

where δ is the Kronecker function, θ is the Heavyside function, q is smooth on $[0,m]$,

$$\int_0^m\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\delta(x)\delta(y)q(z)\mathrm{d}x\mathrm{d}y\mathrm{d}z = \mu = \text{const.}$$

Initially, the ground is not polluted:

$$c(x,y,z,0)=0,\ -\infty<x,y<\infty,\ 0<z<m.$$

The boundary planes are completely impermeable, that is

$$\left.\frac{\partial c(x,y,z,t)}{\partial z}\right|_{z=0}=0,\ \left.\frac{\partial c(x,y,z,t)}{\partial z}\right|_{z=m}= 0,\ t>0,-\infty<x,y<\infty. \quad (2)$$

The most important simplification in the above model is that the parameters are assumed constant. They do not depend either on the actual concentration or the position. If accepted, the homogeneity of the domain results in a linear problem, with the global behavior of the solution contradicting experience. In reality, the pollution runs over only with a finite speed and only a part of the domain becomes polluted, while in the model the pollution immediately appears everywhere. However, in the relative vicinity of the source, the homogeneity may be taken for granted, at least at the first stage of modelling.

The initial boundary problem could be solved by the standard Fourier method using the expansion of the function $q(z)$:

$$c(x,y,z,t)= \mathrm{c}\times\left\{\frac{q_0}{2}\int_0^{\min(t,T)}\frac{1}{t-\tau}\exp[-\lambda(t-\tau)]\right.$$
$$\left.\exp\left\{-\frac{R}{4v_x(t-\tau)}\left[\frac{\left(x-\frac{v_x(t-\tau)}{R}\right)^2}{\alpha_L}+\frac{y^2}{\alpha_T}\right]\right\}\mathrm{d}\tau+ \quad (3)$$
$$\sum_{k=1}^{\infty}q_k\cos\frac{k\pi}{m}z\times\int_0^{\min(t,T)}\frac{1}{t-\tau}\exp[-\lambda_k(t-\tau)]$$
$$\left.\exp\left\{-\frac{R}{4v_x(t-\tau)}\left[\frac{\left(x-\frac{v_x(t-\tau)}{R}\right)^2}{\alpha_L}+\frac{y^2}{\alpha_T}\right]\right\}\mathrm{d}\tau\right\}$$

where

$$c=1/(4\pi v_x n_0\sqrt{\alpha_L\alpha_T}),\ \lambda_k=\lambda+\alpha_T v_x\left(\frac{k\pi}{m}\right)^2,\ \mathrm{k}=1,...,$$

$$q(z)=\frac{q_0}{2}+\sum_{k=0}^{\infty}q_k\cos\frac{k\pi}{m}z,$$
$$q_k=\frac{2}{m}\int_0^m q(z)\cos\frac{k\pi}{m}z\mathrm{d}z,\ k=0,1,... .$$

In the parameter range characteristic for our problem, the very first term dominates the later ones in the Fourier expansion. On the other hand, this term itself appears as a solution of a two-dimensional problem posed for the average of the concentration depth. In order to verify this claim, let us denote the average concentration by C:

$$C(x,y,t)=\frac{1}{m}\int_0^m c(x,y,z,t)\mathrm{d}z$$

and let φ be the average value of the source along the z axis:

$$\varphi(x,y,t)=\frac{1}{m}\delta(x)\delta(y)(\theta(t)-\theta(t-T))\int_0^m q(z)\mathrm{d}z=$$
$$\frac{q_0}{2}\delta(x)\delta(y)(\theta(t)-\theta(t-T)),\ t>0,-\infty<x,y<\infty. \quad (4)$$

If (1) is integrated along the depth z and (2) is taken into account, we arrive at an initial value problem for the equation containing two space variables:

$$Rn_0C_t+v_xC_x=\alpha_Lv_xC_{xx}+\alpha_Tv_xC_{yy}-\lambda Rn_0C+\varphi(x,y,t) \quad (5)$$

with initial value

$$C(x,y,0)=0,\ -\infty<x,y<\infty.$$

The solution is of the form

$$C(x,y,t)=c\,\frac{q_0}{2}\int_0^{\min(t,T)}\frac{1}{t-\tau}\exp[-\lambda(t-\tau)]$$
$$\left.\exp\left\{-\frac{R}{4v_x(t-\tau)}\left[\frac{\left(x-\frac{v_x(t-\tau)}{R}\right)^2}{\alpha_L}+\frac{y^2}{\alpha_T}\right]\right\}\mathrm{d}\tau. \quad (6)$$

Table 2 | Regional parameters

		Source point at			
Parameter	**Dimension**	**Gyál**	**Taksony**	**Apc**	**Dunaharaszti**
Duration	d	90	90	90	60
Thickness of layer (m)	m	20	10	20	5
Infiltration speed (v_x)	m/d	1.5	1.0	1.5	0.2
Porosity (n_0)	—	0.15	0.25	0.15	0.23
Longitudinal dispersity (α_L)	m	25	25	25	15
Transversal dispersity (α_T)	m	0.5	1	1	1.5
Delay factor (R)	—	1.2	1.2	1.2	1.2
Decay rate (λ)	—	0.0001	0	0	0
Prevailing direction (x axis)	—	W–SW	S	E–SE	SW

It is worth noting that, in this formula, $\mu = \frac{1}{2} q_0 m$ is the total source production in unit time. In reality, the value of μ characterizes an extreme situation. Further on, in formula (6) we will use rather μ than q_0.

The approximate value of the concentration can be obtained by any composed quadrature rule. For a small relative error, a uniform partition combined with a simple integration formula calls for a dense grid. Basically, in our calculations we used both the composed trapezoidal rule and midpoint rule with a fixed number $\tilde{N}$ of subintervals. Tests by Romberg iteration showed that, for integer values t and T, the convenient choices $\tilde{N} = Nt_m$, $t_m = \min(t,T)$ and $N = 1$ are sufficient. In this case, the formulae are

$$C(x,y,t) = c\,\frac{\mu}{m}\sum_{i=0}^{t_m} k_i \xi(x,y,t,i), \qquad k_1 = k_{t_m} = \frac{1}{2},$$

otherwise $k_i = 1$

for the trapezoidal rule and

$$C(x,y,t) = c\,\frac{\mu}{m}\sum_{i=1}^{t_m} \xi\left(x,y,t,i-\frac{1}{2}\right)$$

for the midpoint rule. Here $\xi(x,y,t,\tau)$ is the integrand in (6) and note that $\xi(t)$ is replaced by $\lim_{\tau \to t} \xi(t)$ in the trapezoidal rule.

For the relative accuracy $\varepsilon = 10^{-5}$, the computational costs became smaller by two orders when a higher order formula (an eight-point Newton–Cotes quadrature) and an adaptive automatic selection of subinterval length were applied. For verification of the numerical results, including the check of dependency on parameters, we applied formulae of this type.

PARAMETER SELECTION, SENSITIVITY AND NUMERICAL RESULTS

When assigning parameter values, the least difficulties occur with the constant production of the pollution μ and with the thickness m of the layer. Both quantities appear in (6) as multipliers. The same holds for the porosity n_0.

The infiltration speed is taken equal to the speed of the groundwater flow. This assumption is acceptable until the concentration reaches a high value.

Table 3 | Maximal concentrations versus distance

Distance	Number of days	Max. concentration
200	90	0.0029
400	240	0.0014
600	400	0.00092
800	560	0.00067
1000	710	0.00053

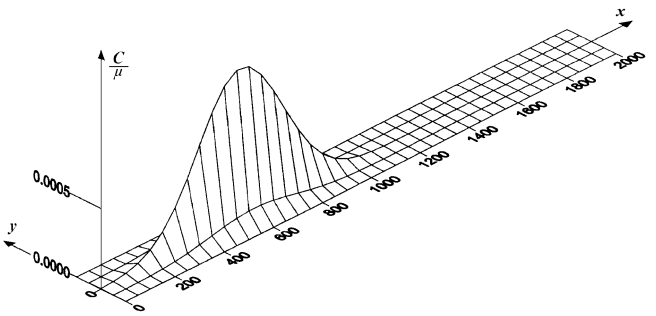

Figure 1 | Pollution wave at waste material depository, Gyál, 500 days after the break down.

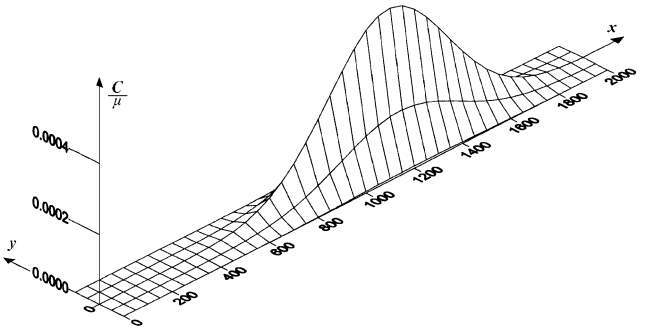

Figure 2 | Pollution wave at waste material depository, Gyál, 1000 days after the break down.

As concerns the dispersities, we could rely upon the estimates of the local experts. The pollution source is assumed to be active at most between two consequent monitoring dates, i.e. the period of activity is 30, 60 or 90 days. As we stated previously, during this period the production is assumed to be uniform. Due to the uncertainty in the parameters, we checked the sensitivity of the concentration with respect to the parameters occurring in (6) non-linearly. The main point was sensitivity with respect to the ratio $\alpha = \alpha_L/\alpha_T$. While α_L is relatively well known, this is not the case with α_T. As the experts claim, the measurements give rather the value of α than α_T and with high uncertainty. Along the x axis, α appears as an amplification factor only. In general, however, it has an impact on the shape of the level sets. Together with the maximal value during the observation period, the maximum point is displaced as well. An illustrative example will be given at the end of the next section.

Computations were made for four regions. The parameter set characteristic for the regions is listed in Table 2. The last row contains the prevailing direction of the flow. It is used for locating the coordinate system.

Due to the costs and time restrictions there was no possibility of carrying out either repeated measurements or calibration of data. Instead, we made an intensive computation and a consequent comparison of the results in the range of the parameters (Table 1). The next section contains some results obtained with the data corresponding to Table 2.

POLLUTION MAPS

We wanted to follow the propagation of the pollution in the region where it is most dangerous. Hence, in the prevailing direction of infiltration (x) a relatively large distance was covered by the computation, while in the perpendicular direction a shorter distance was chosen. When the homogeneity took place, the concentration was computed over a rectangular grid in the domain

$$0 \le x \le 2000, \quad -100 \le y \le 100. \tag{7}$$

We recall that the model is valid until homogeneity is not violated. Thus, the impact caused by a river, an artificial channel or a lake required additional analysis. This was the case near Apc due to the brook Szuha and also at Dunaharaszti where the Danube–Tisza Channel is located. In the first case, we could neglect the presence of

Table 4 | Maximal concentrations versus time

Number of days	Maximal concentration	Location of the maximum (m)
100	0.0090	50
200	0.0027	200
300	0.0017	300
400	0.0012	450
500	0.00093	550
600	0.00076	700
700	0.00063	800
800	0.00055	950
900	0.00048	1050
1000	0.00042	1200
1100	0.00038	1300
1200	0.00034	1450

the Szuha because it is very small. In the second case, we suggested a more rigorous monitoring, ensuring that the groundwater pollution with a significant concentration could not reach the vicinity of the channel.

We now describe some tables and maps provided by our simulation model and suitable for the evaluation of a mishap.

Worst-case study

The maximal concentration values along the x axis were found at the distances given in the first column of Table 3. They occurred $\tilde{t}$ days after the operational mishap was assumed to be noticed and stopped (at $T = 90$ days). The second column contains the values $\tilde{t}$. The maximal concentration value itself is given in the third column ($\mu = 1$). The data are given for the region of Gyál. A post-mishap situation is simulated there.

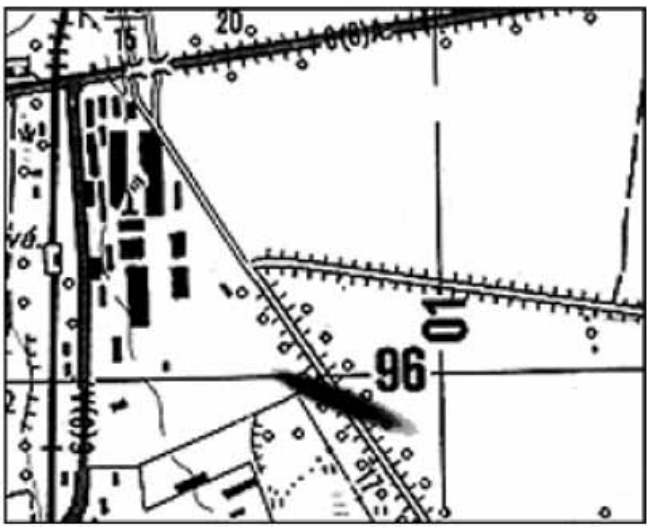

Figure 3 | Estimated soil water pollution at aluminium smeltery, Apc, 100 days after the break down.

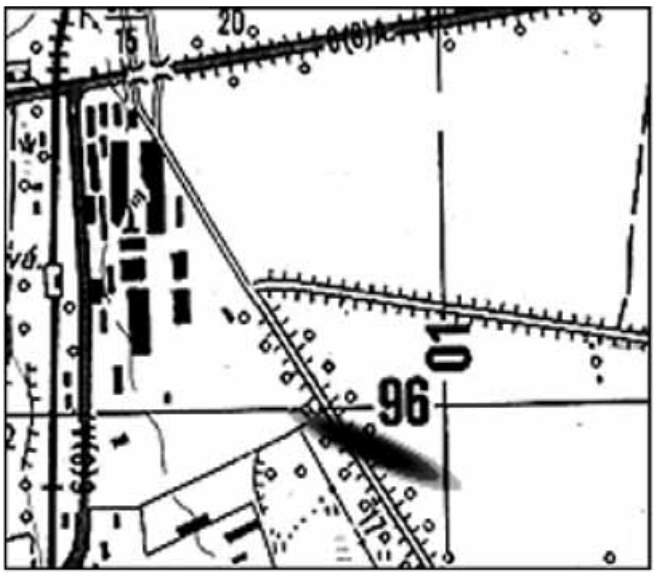

Figure 4 | Estimated soil water pollution at aluminium smeltery, Apc, 150 days after the break down.

Time dependence of the distribution of the pollution (in region (7))

Three-dimensional plots drawn from the data show the post-mishap distribution at $t = 100, 200, \ldots, 1200$ days. Two of these maps for the Gyál region are given in Figures 1 and 2.

Table 5 | Dependence of the concentration on the dispersity

Case (a) Longitudinal dispersity=15.0, transversal dispersity=1.5

	Second coordinate (perpendicular to the prevailing direction)					
Number of days	**0 m**	**±10 m**	**±20 m**	**±30 m**	**±40 m**	**±50 m**
380	7.754E-3	5.872E-3	2.553E-3	0.640E-3	0.93E-4	0.8E-5
390	7.916E-3	6.041E-3	2.688E-3	0.699E-3	1.07E-4	1.0E-5
400	8.055E-3	6.192E-3	2.815E-3	0.759E-3	1.22E-4	1.2E-5
410	8.170E-3	6.324E-3	2.934E-3	0.818E-3	1.38E-4	1.4E-5
420	8.263E-3	6.438E-3	3.046E-3	0.877E-3	1.54E-4	1.7E-5
430	8.336E-3	6.535E-3	3.150E-3	0.936E-3	1.72E-4	2.0E-5
440	8.389E-3	6.615E-3	3.246E-3	0.993E-3	1.90E-4	2.3E-5
450	8.423E-3	6.679E-3	3.333E-3	1.048E-3	2.08E-4	2.6E-5
460	8.440E-3	6.729E-3	3.412E-3	1.102E-3	2.27E-4	3.0E-5
470	8.440E-3	6.764E-3	3.483E-3	1.154E-3	2.47E-4	3.4E-5
480	8.426E-3	6.786E-3	3.546E-3	1.204E-3	2.66E-4	3.8E-5
490	8.398E-3	6.795E-3	3.601E-3	1.251E-3	2.86E-4	4.3E-5
500	8.357E-3	6.792E-3	3.648E-3	1.296E-3	3.05E-4	4.8E-5
Case (b) Longitudinal dispersity=25.0, transversal dispersity=1.0						
380	8.808E-3	5.801E-3	1.661E-3	2.09E-4	1.2E-5	0
390	8.819E-3	5.876E-3	1.742E-3	2.31E-4	1.4E-5	0
400	8.815E-3	5.938E-3	1.819E-3	2.55E-4	1.6E-5	0
410	8.797E-3	5.987E-3	1.891E-3	2.79E-4	1.9E-5	1E-6
420	8.766E-3	6.025E-3	1.960E-3	3.03E-4	2.3E-5	1E-6
430	8.723E-3	6.053E-3	2.025E-3	3.28E-4	2.6E-5	1E-6
440	8.671E-3	6.070E-3	2.085E-3	3.53E-4	3.0E-5	1E-6
450	8.609E-3	6.078E-3	2.142E-3	3.78E-4	3.4E-5	2E-6
460	8.538E-3	6.077E-3	2.194E-3	4.03E-4	3.8E-5	2E-6
470	8.461E-3	6.069E-3	2.242E-3	4.28E-4	4.2E-5	2E-6
480	8.376E-3	6.053E-3	2.286E-3	4.53E-4	4.7E-5	3E-6
490	8.286E-3	6.030E-3	2.326E-3	4.77E-4	5.2E-5	3E-6
500	8.191E-3	6.002E-3	2.362E-3	5.01E-4	5.7E-5	4E-6

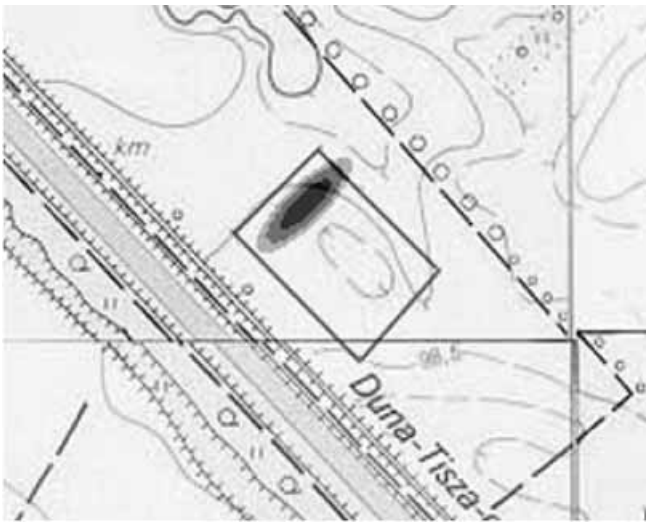

Figure 5 | Plant, Dunaharaszti, 470 days after the break down.

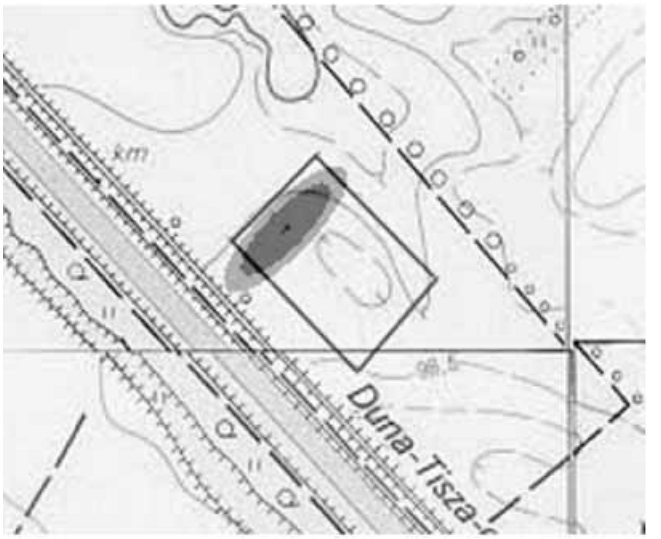

Figure 6 | Plant, Dunaharaszti, 700 days after the break down.

The figures are scaled adaptively. For more transparency, the locations and the values of the maximal concentrations at fixed time values were extracted from the plots and supplied in Table 4.

Direct in-time decisions

Coloured maps were drawn for specific components of the pollution. At Apc an aluminium smeltery is in operation. An accident may cause pollution of the region by hazardous chemicals including As, Ba, Cd, Co, Cr, Cu, Hg, K, Mo, Ni, Pb, Zn, cyanids, etc. For most of them predictions were computed and the results were shown on separate coloured maps. The value ranges for the colours were chosen for each component relative to their load limits and intervention limits. Figures 3 and 4 illustrate the maps in a black and white version.

Sensitivity analysis

The impact of the uncertainty in parameters α_L and α_T requires special attention at Dunaharaszti, where the composting plant is close to the Danube–Tisza Channel (the distance is 125 m). As we mentioned before, the model is not valid near the channel. Therefore we compare the concentrations for different parameter values on a line separating the composting plant and the channel. The shortest distance between them is divided in the ratio 1:4. The groundwater flow is perpendicular to the flow in the channel. Thus the highest concentration along the line is at the point $(x,y) = (100.0)$. Results in the neighbourhood of this point at the line parallel to the channel, i.e. for $-50 < y < 50$ and for time values relatively close to the moment when the concentration is maximal at the given point, are tabulated for two equally possible parameter pairs (α_L, α_T), see Table 5. To compare with the given load limits, we resized the concentration computed for $\mu = 1$. The results become very expressive in coloured maps. Here, black and white versions are supplied as Figures 5 and 6.

CONCLUSION

A relatively simple transport equation modelling the spread of pollutants in groundwater was used for evaluation of the possible damage to the environment. An extensive analysis of the numerical results accompanied by visualization convinced us in the applicability of the

models for four regions in Hungary. Based on the analysis, we could give a sufficiently reliable forecast at a relatively low computational cost.

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