Quality of Groundwater, Proceedings of an International Symposium, Noordwijkerhout, 849
The Netherlands, 23–27 March 1981, W. van Duijvenbooden, P. Glasbergen and H. van Lelyveld (Eds.),
Studies in Environmental Science, Volume 17

TWO- AND THREEDIMENSIONAL MATHEMATICAL MODELS OF CONTAMINANT MOVEMENT IN GROUNDWATER

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ABSTRACT

The application of a 3-dimensional transport model is limited because of computer size and costs. Therefore it will be necessary to make simplifying approximations. Two models are presented, a 3-dimensional model with a homogeneous flow-field, which can be used in the vicinity of locally limited sources, and a 2-dimensional model for extended aquifers with different size and direction of groundwater flow.

INTRODUCTION

Investigation and management of groundwater is one of the most important tasks of water resources research. Because of industrial and agricultural activities an increasing loss of groundwater quality can be observed. Besides budget calculations more and more attention has to be payed to the quality of groundwater resources. Methods need to be developped to predict the effects of artificially induced and natural groundwater contaminations to protect groundwater supplies from further impairment.

Specifically, mathematical simulation models are well suited to help solving these problems. Two examples are introduced to demonstrate the applicability of transport models in groundwater flow.

THEORY

The mathematical description of mass transport in flowing groundwater is based on two partial differential equations: first, the equation of flow, from which the groundwater velocities are obtained, and second, the solute-transport equation, describing the change of the chemical concentration in the groundwater.

FLOW EQUATION

The partial differential equation of groundwater flow in a slightly confined aquifer in three dimensions may be written as (ref. 1)

$$s \cdot \frac{\partial h}{\partial t} = \mathrm{div}(k_f \cdot \mathrm{grad}\ h\ ) \pm q \tag{1}$$

where h = hydraulic head
s = specific yield (storage)
k_f = permeability tensor
±q = volumetric flux of re-(+) or discharge (-)
(source(+) or sink(-) term)

Following Darcy's law the average seepage velocity of groundwater can be determined from the head distribution.

$$\vec{v} = -(k_f/n) \cdot \mathrm{grad}\ h \tag{2}$$

where $\vec{v}$ = seepage velocity (mean pore velocity)
n = effective porosity

TRANSPORT EQUATION

The equation used to describe transport and dispersion of dissolved substances in flowing groundwater is (ref. 1, 2)

$$\frac{\partial c}{\partial t} = \mathrm{div}(\ D \cdot \mathrm{grad}\ c\ -\ \vec{v} \cdot c\ )\ -\ r \tag{3}$$

where c = concentration of dissolved material
D = diffusion-dispersion tensor
$\vec{v}$ = mean pore velocity
r = rate of sorption of the species due to
physical adsorption or chemical reactions

The first term on the right hand side describes the change of concentration due to hydrodynamic diffusion and dispersion. The second term represents the convective transport, while the third term, in the mathematical sense a source or sink, considers the effects of ad- and desorption and chemical reactions. This can be neglected for the case of nonreacting species.

NUMERICAL METHODS

Commenly three general classes of numerical methods are used to solve partial differential equations: finite-difference methods, finite-element methods and the method of characteristics. Each method has some advantages, disadvantages and special limitations for applications to field problems.

In this study a finite-difference method was prefered. Maybe, this method has some disadvantages in view of flexibility of the grid size, memory requirements, choice of the time step, etc., but it is the simplest method, mathematically, and the easiest to program for a digital computer.

The finite-difference form, applied to the flow equation was an implicit, block-centered difference scheme, solved by an iterative procedure (SOR). For the transport equation the CRANK-NICOLSON method was chosen. In comparison to a strongly implicit scheme this method is more effective. To prevent overshooting and inaccurate results the increments of time and space must be chosen so that

$$\max\ (\Delta x_i/\alpha_i) \lesssim 2 \quad \text{and} \quad \max\ (v_i \cdot \Delta t/\Delta x_i) \lesssim 2$$

where Δt time-, Δx_i space increment, α_i dispersivity, v_i velocity in i-direction.

MODELLING FIELD PROBLEMS

The application of a three dimensional model is limited because of computer size and costs. Table 1 shows the dependency of memory requirement and the grid size for a 1-,2-,and a 3-dimensional model. Because of the immense increase of memory requirements it will be always necessary to make some simplifying approximations.

TABLE 1

Memory requirement for the transport model

	dimension		
field	1	2	3
velocity	1 * i	2 * (i*j)	3 * (i*j*k)
dispersion	1 * i	3 * (i*j)	6 * (i*j*k)
concentration	2 * i	2 * (i*j)	2 • (i*j*k)
total	4 * i	7 • (i*j)	11 * (i*j*k)

i,j,k = number of nodes in x-, y- and z-direction

The first example chosen, shows the spreading from a line source. In this case it is possible to reduce the dimension by consideration of a vertical section because of the large scale in y-direction.

The problem, which should be solved, was to prevent or diminish the pollution of the groundwater by infiltration from a river. The water of the river has a high content of cloride and sulfate and it was observed that during flood periods these substances infiltrate into the groundwater aquifer.

First the flow-field was calculated. The aquifer was assumed to be homogeneous and isotropic with an average permeability of $k_f = 5 \cdot 10^{-4}$ m/s. The area of interest was divided by a rectangular grid of 65 • 15 = 975 node-points for which the hydraulic head and the components of flow in x- and y-direction were calculated.

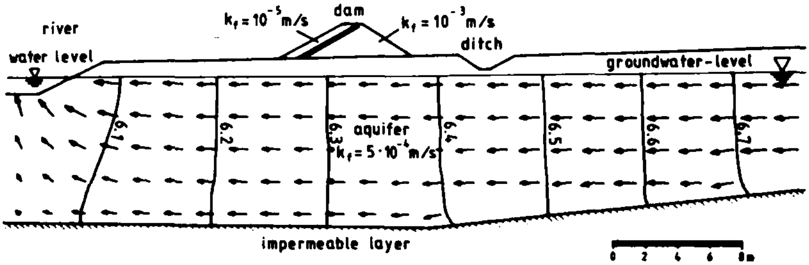

Fig. 1. Potential- and streamlines of groundwater flow computed for a normal river water level

Fig. (1) shows the normal case. Assuming steady state conditions and an average stream flow all ground water is directed to the river. The situation changes for a flood. Fig. (2) shows the flow field for a 10-year flood. The direction of groundwater flow has turned. Polluted river water now infiltrates into the groundwater. A drainage ditch behind the dam prevents the extension into the hinterland.

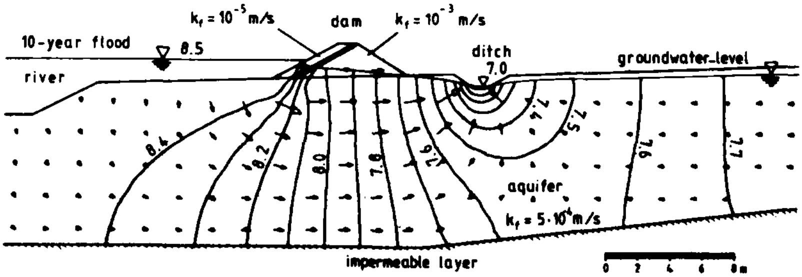

Fig. 2. Potential- and streamlines of groundwater flow computed for a 10-year flood

The transport model was used to compute the chloride concentration during the flood period. According to table 1, 7*975 = 6825 words memory size are needed for computing the concentration of the 975 nodes. Fig. (3) shows the groundwater contamination 2 days after the beginning of the flood. The chloride-front has reached the ditch; 8 days later (Fig. (4)) the section between the river and the ditch is totally contaminated with chloride. The effectiveness of the drainage ditch is obvious. The chloride-zone ends about 4 to 5 m behind the ditch.

After 10 days the flood is over and we have normal conditions. The groundwater flow is directed towards the river again and the chloride bearing water gradually is displaced by fresh water (Fig. 5 and Fig. 6). 10 days after the flood most of the chloride has been refluxed towards the river.

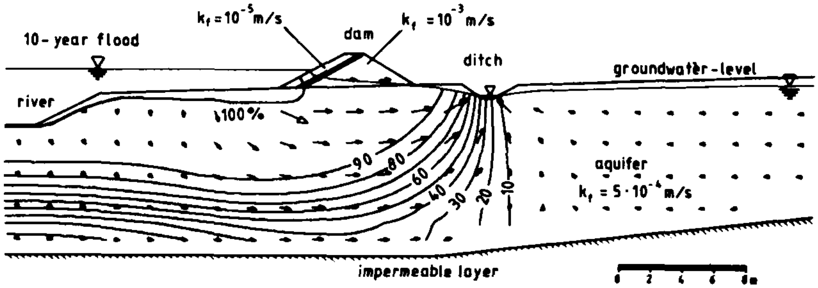

Fig. 3. Relative concentrations computed 2 days after the beginning of the flood.

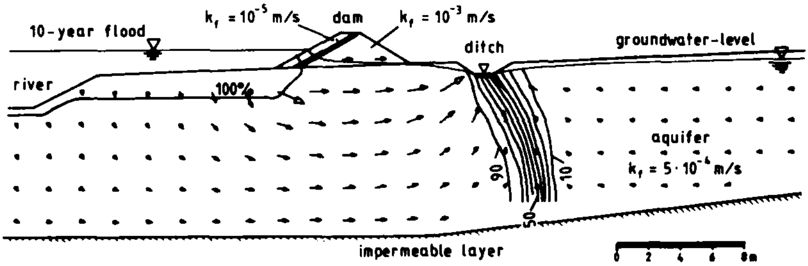

Fig. 4. Relative concentrations computed 10 days after the beginning of the flood.

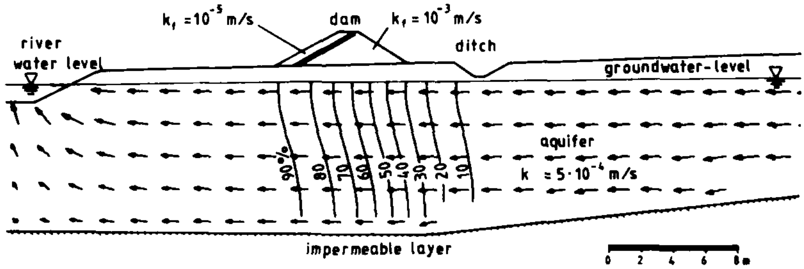

Fig. 5. Relative concentrations computed 2 days after the end of the flood.

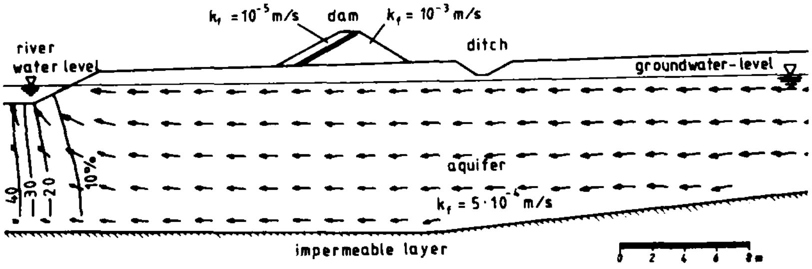

Fig. 6. Relative concentrations computed 10 days after the end of the flood.

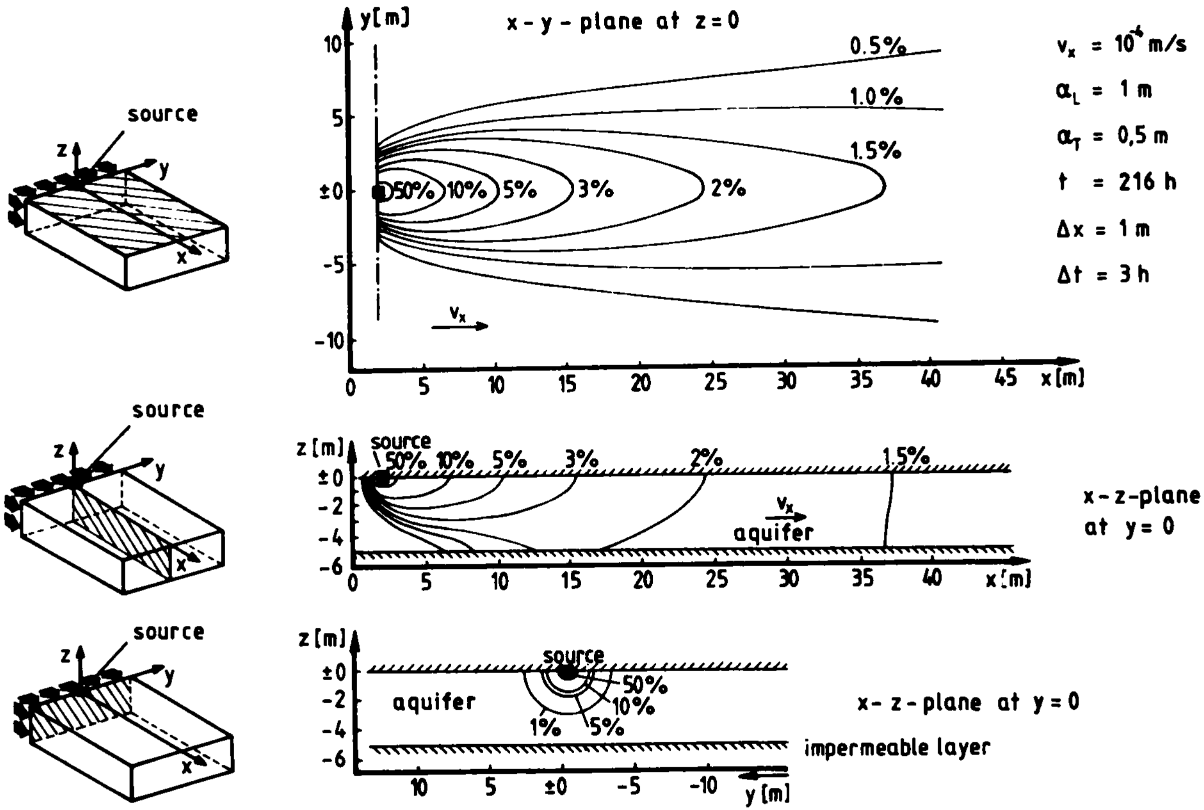

Fig. 7. Groundwater contamination in the vicinity of a point source computed after 9 days.

The second example shows the spreading from a point source. The source, for example a waste disposal, is located on top of an aquifer, which vertically is limited by an impermeable layer. For this problem a 3-dimensional description is needed. If the horizontal dimension of the groundwater flow can be stated as being very large, vertical flow can be neclected. Furthermore, the horizontal flow direction does not change significantly in the vicinity of the source, so that a flow field parallel to the x-axis can be assumed. In this case the model needs a memory size of 7 • (40*20*5) = 28 000 words.

Fig.(7) shows the computed groundwater contamination in the close vicinity of the source. After some time, in this case 216 h = 9 days , steady-state conditions are reached for the part looked at. The limitation of the aquifer interrupts the unlimited vertical spreading and leads to a vertical profile constant concentration a certain distance from the source (see x-z plane in Fig.(7)). At this distance it is possible to continue with a 2-dimensional horizontal model, which saves computer size and time as well. The coupling of the 3-dimensional model to the 2-dimensional is easy to realize, because the boundary conditions, which have to be transfered are constant in space and time.

SUMMARY

Groundwater pollution problems can be successfully studied with mathematical transport models, which use finite-difference methods. The application of 3-dimensional models is limited because of computer size and costs. In most cases it is possible to reduce memory requirement and computer time by making some simplifying approximations, which was shown by two examples.

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