

Impact of sedimentary structures with inclined couplets on solute transport in gravel aquifers

FRITZ STAUFFER

Institute of Environmental Engineering, ETH Zurich, CH-8093 Zurich / Switzerland

e-mail: stauffer@ifu.baug.ethz.ch

Abstract Investigations in outcrops of heterogeneous gravel deposits in north-eastern Switzerland by Jussel et al. (1994a) revealed that distinct sedimentary structures appear as more or less horizontal lenses and layers within extended patches of background gravel material. However, two out of the observed facies element types, the open framework/bimodal gravel couplets and part of the combined structures of grey gravel (bimodal gravel without silt) and brown gravel (bimodal gravel with silt), consist of inclined couplets. They are the results of fluvial processes with the filling of troughs and channels. Together, these two facies elements account for about 10% of the sediment volume. Stauffer and Rauber (1998) performed three-dimensional stochastic facies type transport modelling in a uniform mean flow field over a distance of 100m of a saturated aquifer and compared the results with those of analytical stochastic unimodal and bimodal macrodispersion models. In the latter the inclination of couplets is neglected. The bimodal approach clearly showed better correspondence with the numerical stochastic facies modelling results. This was primarily due to the pronounced bimodal probability density of the hydraulic conductivity values, which was observed in the field. However, differences were still present and striking. Can they be attributed to the inclination of the sediment couplets? This inclination manifests itself as a strong anisotropy of the hydraulic conductivity tensor with inclined principal axes of the facies element. In this paper the role of sedimentary structures with inclined couplets is investigated by a series of three-dimensional numerical flow and transport experiments. Single lenses of sedimentary structures with inclined principal axis of the hydraulic conductivity tensor are investigated, which are imbedded in a homogeneous background matrix material. Particle tracking on models with presence of such structures shows pronounced lateral (horizontal and vertical) deflexions. These observations can better explain the results of the stochastic facies modelling of Stauffer and Rauber (1998) in a qualitative manner. The results allow to better understand the transport processes, which are responsible for macrodispersion effects in heterogeneous gravel aquifers at the local scale.

Key words flow, hydraulic conductivity, inhomogeneous, anisotropic, finite element model, advective transport, macrodispersion

INTRODUCTION

The topic of this paper is the investigation of the role of one class of sedimentary structures on the transport of solutes in aquifers. Sedimentary structures of natural sandy gravel deposits in north-eastern Switzerland were described and statistically analyzed by Jussel et al. (1994a). Freshly excavated outcrops in gravel pits revealed distinct sedimentary structures appearing as lenses and layers, mostly embedded in a background gravel matrix. They determined hydraulic properties of the different sedimentary structures (hydraulic conductivity and porosity) in the laboratory from disturbed and undisturbed samples. The data showed large differences in hydraulic conductivity among the different types of sedimentary structures of up to five orders of magnitude.

The gravel material mainly consisted of sandy gravel with silt (grey gravel) and without silt (brown gravel), sand, little silt, and well sorted extremely conductive coarse gravel (open framework gravel). Two sedimentary structures consisted of alternate layers of different materials. One of them is formed by inclined open framework/bimodal gravel couplets. Bimodal gravel material is characterized by its distinctly bimodal grain size distribution. The other structural element consisted of horizontal or inclined brown and grey gravel layers forming extended patches. Fig. 1 shows an example of the detected sedimentary structures from the Huentwangen gravel pit (Rhine valley near Zurich, Switzerland). All structure types were specified by statistical parameters (mean and variance) defining the lens length, the lens height, the direction of the principal axis of the lens with respect to the former flow direction of the sedimenting river, the hydraulic conductivity tensor, the porosity, the local dispersivity, and geostatistical parameters. A weak spatial variability of hydraulic conductivity was present within each single lens of a given type. A much higher variability was found between different lenses of the same type. Eventually, an even wider variability was present between different sedimentary structure types. The open framework gravel material caused the probability density function of log-hydraulic conductivity in the overall gravel material to be bimodal. All other gravel material together approximately fitted a log-normal distribution. Open framework gravel is present as relatively short and thin, horizontal or inclined lenses or group of lenses.

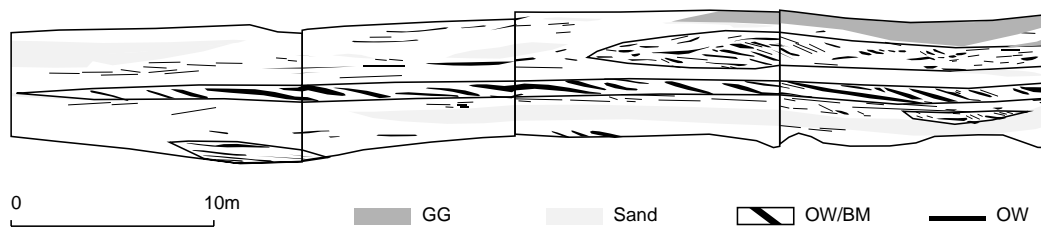


Fig. 1 Sedimentary structures detected in the Huentwangen gravel pit (Rhine valley near Zurich, Switzerland); OW: open framework gravel; BM: bimodal gravel; GG: grey gravel; the background gravel consist of GG/BM and BG (brown gravel) structures, which are not distinguished in the graph (after Stauffer and Rauber, 1998).

Jussel et al. (1994b) and Stauffer and Rauber (1998) used the detailed statistical information on facies geometry and the hydraulic parameters to numerically generate unconditional realizations of synthetic block-shaped facies type aquifers. They assumed that the structure elements ‘grey gravel’, ‘brown gravel’ and mixtures of both (layered or not) represent the matrix, in which lens type elements (single open framework gravel lenses, sand lenses, open framework-bimodal gravel couplets, inclined grey gravel/brown gravel couplets, and silt lenses) are embedded. A lens shape is approximated in their model by an ellipse in the plan view and by a power function in the vertical cross section. They generated the facies in their unconditional model as follows:

1. Generation of the matrix-type sedimentary structures. While the grey gravel/brown gravel structure was considered as the background matrix, pure grey gravel and brown gravel lenses were treated as matrix-type lenses, thus embedded in the background matrix. They were generated by defining the position and the size of each lens. These elements were randomly set allowing no overlapping of lenses.

2. Generation of the lens-type sedimentary structures by defining the position and the size of each lens. Again these lenses were set at random, excluding any overlapping regions.
3. The geometric mean hydraulic conductivity values of the lenses of a given sedimentary structure type were randomly chosen according to the corresponding global mean and variance. Assignment of porosity and local dispersivity values for a given structure type.
4. Assignment of a correlated field of log-hydraulic conductivity within each structure element according to the selected mean and the variance.

The model for three-dimensional, saturated steady-state flow is based on the flow continuity equation

$$\nabla \cdot (\mathbf{K} \nabla h) = 0 \quad (1)$$

where \mathbf{K} is the hydraulic conductivity tensor and h is the head. Boundary conditions taken into account were either prescribed head or impermeable boundary. Stauffer and Rauber (1998) integrated the flow equation by using the Finite Element method. The local matrices of the three-dimensional finite elements were calculated by using isoparametric hexahedral elements with trilinear shape functions. A block sized model domain was subdivided into hexahedral finite elements. Starting from a regular pattern of prismatic elements with rectangular cross section, each element in the model domain could be distorted in order to reproduce the typical lens-shape geometry. The flow calculation yielded the specific flux field in the entire model domain. The three-dimensional transport model was based on the mass balance equation for a conservative solute, which accounted for the effect of advection and dispersion. The equation was numerically integrated by the Random Walk method. Stauffer and Rauber (1998) performed stochastic numerical flow and transport experiments using 100 different synthetic block shaped gravel aquifers of the size 110m in x -, 35m in y -, and 6m in z -direction. On the inflow surface at $x=0$ the hydraulic head was fixed at $h=0.55$ m, and on the outflow surface at $x=110$ m, it was set to $h=0$. All other surfaces were impermeable. The flow domain was discretised by $110 \times 35 \times 60$ finite elements. The elements were distorted by matching the actual lens shape. The tracer transport problem consisted of observing the evolution of the moments of a tracer cloud represented by 2000 mass particles initially located at $x=5$ m in a finite vertical area of the size 5m x 2m perpendicular to the mean flow. Apparent macrodispersivity values (longitudinal, transversal horizontal, and transversal vertical) were estimated by analyzing the moments and the breakthrough of the tracer cloud at different locations x according to the method as described by Jussel et al. (1994b). Results are shown in Fig. 2.

Stauffer and Rauber (1998) used the statistical parameters of the sedimentary structures to characterize the overall gravel deposit by a single variance and a single correlation length of log-hydraulic conductivity. These parameters (variance and correlation length of log-hydraulic conductivity) were directly applied to an analytical unimodal stochastic model of apparent macrodispersivity according to Dagan (1988). The results are also shown in Fig. 2 for comparison with the numerical results. Compared to the numerical results large discrepancies are present.

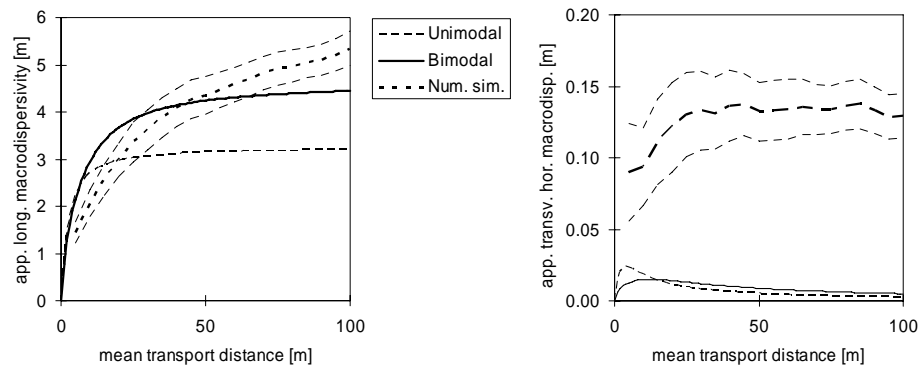


Fig. 2 Apparent longitudinal (left) and transversal horizontal (right) macrodispersivity over mean transport distance x from stochastic facies modelling. The 95% confidence intervals of the numerical results are shown as dashed lines (after Stauffer and Rauber, 1998).

In order to account for the bimodal nature of the probability density of hydraulic conductivity, Stauffer and Rauber (1998) developed an analytical anisotropic stochastic model. In a bimodal heterogeneous porous medium lens type inclusions with open framework material of a given volumetric fraction were considered in a background material consisting of all material except open framework material. These inclusions were defined by their volumetric fraction and their anisotropic (horizontal and vertical) indicator variogram, which was based on observations in the gravel pit. Therefore, the inclusions were statistically distributed within the background matrix, but all lenses essentially had to be horizontal. Stauffer and Rauber (1998) found that both the unimodal and the bimodal approach were not in satisfactory agreement with the numerical stochastic facies modelling results. The differences may be attributed to the existence of open framework/bimodal couplets with inclined bedding since the effect of inclined bedding could not be taken into account in the analytical bimodal approach.

In this paper the role of sedimentary structures with inclined open framework/bimodal couplets on flow and solute transport is investigated by a series of three-dimensional numerical flow and transport experiments. A single anisotropic, highly permeable lens is investigated, which is imbedded in homogeneous background matrix material. The inclined bedding of the lens is modelled in an averaged manner by an inclined principal axis of the hydraulic conductivity tensor. The results should allow to better understand the transport phenomena, which are responsible for the macrodispersion development in heterogeneous gravel aquifers at the local scale (scale of 100m).

NUMERICAL MODEL FOR A SINGLE EMBEDDED LENS IN A BACKGROUND MATRIX

For this study the flow equation is integrated by the Finite Element method. The local matrices of the finite elements are calculated by using three-dimensional isoparametric hexahedral elements with trilinear shape functions as used by Stauffer and Rauber (1998). A block sized model domain is subdivided into a regular pattern of prismatic finite elements. The flow calculation yields the specific flux field in the entire model domain. The three-dimensional transport equation is numerically approximated by the particle tracking method thus disregarding molecular diffusion and mechanical dispersion. The code is written in FORTRAN for a PC with processors Intel Pentium 4 CPU 2.4 GHz.

The synthetic block-shaped gravel aquifer is of the size $L_x=110\text{m}$, $L_y=36\text{m}$, and $L_z=6\text{m}$. On the inflow face at $x=0$ the hydraulic head is fixed to $h=0.55\text{m}$, and on the outflow face at $x=110\text{m}$, it is set to $h=0$. All other surfaces are impermeable. The flow domain is discretised by $110 \times 36 \times 60$ finite elements. Therefore, the model domain is practically identical to that used by Stauffer and Rauber (1998). The horizontal background hydraulic conductivity is $K_{\text{hor}}=2.0 \cdot 10^{-4} \text{ m s}^{-1}$ and the vertical hydraulic conductivity is $K_{\text{vert}}=2.0 \cdot 10^{-4} \text{ m s}^{-1}$ (isotropic case) and $2.0 \cdot 10^{-5} \text{ m s}^{-1}$ (anisotropic case). Therefore, an isotropic model domain and an anisotropic model domain with horizontal principal direction of the hydraulic conductivity tensor are considered as background. In this model domain, a single lens of length $l_x=20 \text{ m}$, width $l_y=10 \text{ m}$, and thickness $l_z=1\text{m}$, is embedded in the centre of the flow domain (Fig. 3). The maximum hydraulic conductivity in the anisotropic lens is $K_{\text{lens,max}}=0.01 \text{ m s}^{-1}$ and the minimum value is $K_{\text{lens,min}}=2.5 \cdot 10^{-4} \text{ m s}^{-1}$. The horizontal angle of the principal direction of the hydraulic conductivity tensor with respect to the x -axis is chosen from the interval $\kappa=0$ to $\pi/2$ (rad). The Inclination of this principal direction or plane with maximum hydraulic conductivity is selected to $\psi=0$ and $\psi=-0.332$ (rad) with respect to the horizontal plane. Porosity was chosen as $\phi=0.2$. All parameters and conditions are identical or close to those used by Stauffer and Rauber (1998). The anisotropic single lens corresponds to a typical open framework/bimodal couplets. The inclined layering is represented in an averaged manner by an anisotropic hydraulic conductivity tensor due to discretisation reasons. The horizontal angle and the inclination of the principal direction of the hydraulic conductivity tensor correspond to typical direction and inclination of the layering as observed in the field.

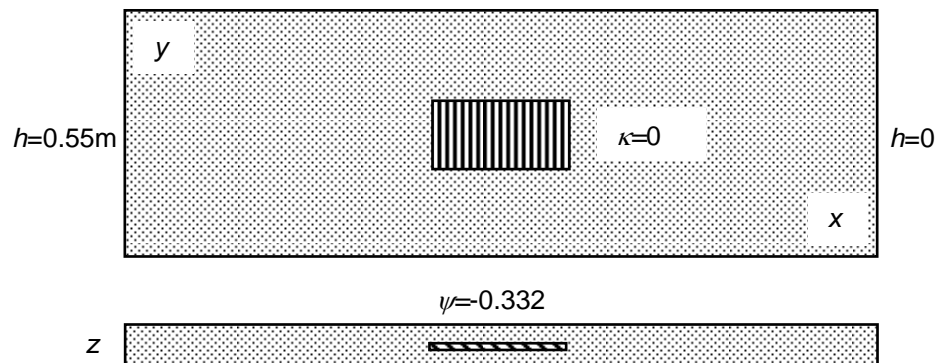


Fig. 3 Block-sized model domain with plan view (above) and cross section (below). Fixed head boundary condition at $x=0$ (inflow face) and $x=110\text{m}$ (outflow face). Single lens ($20\text{m} \times 10\text{m} \times 1\text{m}$) with angle κ and inclination ψ of the principal direction of anisotropy is located in the centre.

For each of the parameter configurations defined above the three-dimensional head field is determined. Based on these fields solute transport is modelled by using the Particle Tracking technique. For this purpose the particles of a dense vertical array (36×60 particles according to element centres at the inflow face) are marked by their lateral (y -) and vertical (z -) coordinates. Isolines are evaluated for both the initial y - and the z -values of the particles. With this technique vertical and horizontal stripe-shaped features can be visualized in the inflow profile. The width of the stripes was selected to 1m horizontally and to 0.5m vertically. Caused by the single lens, the corresponding pattern in the outflow profile may be disturbed thus showing up in a distorted outflow pattern. The inflow and outflow patterns are thus cuts to streamtubes.

Analyzing outflow streamtubes for the selected configuration makes sense especially for the case that all particle tracks close to the outflow face are practically parallel to the x-axis. This property was checked beforehand. Furthermore, a measure for the distortion of the streamtubes in the outflow face is formulated. It was taken as the sum of the weighted squared vertical deviations

$$S_z = \sum (\Delta z)^2 \Delta V \quad (2)$$

and as weighted squared horizontal deviations

$$S_y = \sum (\Delta y)^2 \Delta V \quad (3)$$

where the sum is taken over the particles in all element centres close to the inflow face weighted with the volume ΔV of the corresponding finite element. Δz and Δy are vertical and horizontal deviations in the outflow face with respect to the location for the particle trajectory without lens.

RESULTS

Inflow streamtube patterns of all cases are equidistant parallel vertical or horizontal stripes. The outflow streamtube pattern of an isotropic lens, or of an anisotropic lens with inclination $\psi=0$, or anisotropic lens with horizontal angle $\kappa=\pi/2$ are identical or practically identical with the corresponding inflow patterns. As expected, no or almost no distortion effect was observed in these lenses. This holds true also for anisotropic matrices. Vertical and horizontal patterns of streamtubes at the outflow face at $x=110\text{m}$ for the isotropic and the anisotropic matrix with anisotropic embedded single anisotropic lens with horizontal angle $\kappa=0$, and $\kappa=\pi/4$ and with inclination $\psi=-0.332$ are shown in Fig. 4 to 7. The sum of weighted squared vertical and horizontal deviations of the particles is shown in Fig. 8 and 9. Finally, selected particle tracks for isotropic and anisotropic matrix with horizontal angle $\kappa=\pi/4$ are shown in Fig. 10 and 11.

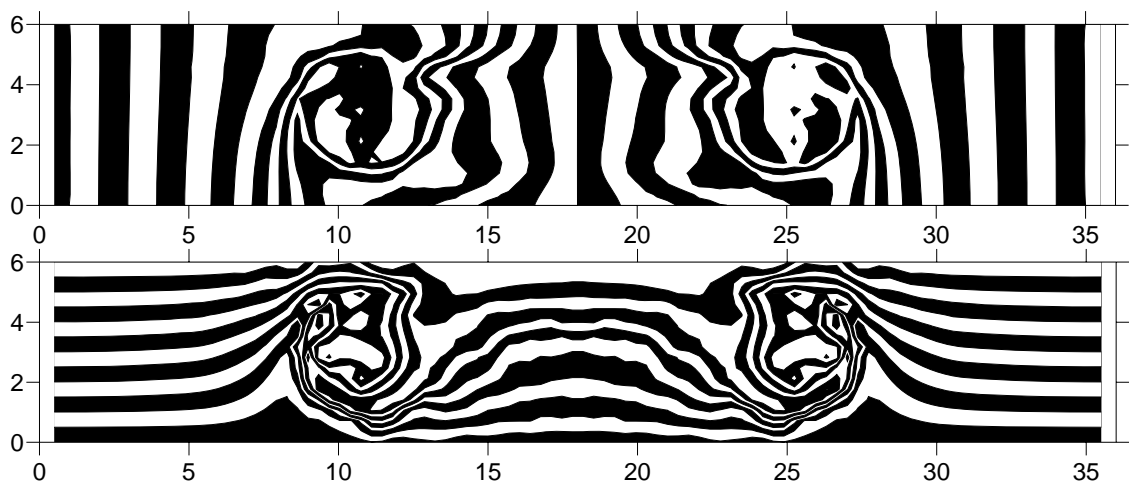


Fig. 4 Outflow streamtube pattern from vertical (above) and horizontal (below) inflow pattern for isotropic matrix with anisotropic single lens with $\kappa=0$, and $\psi=-0.332$.

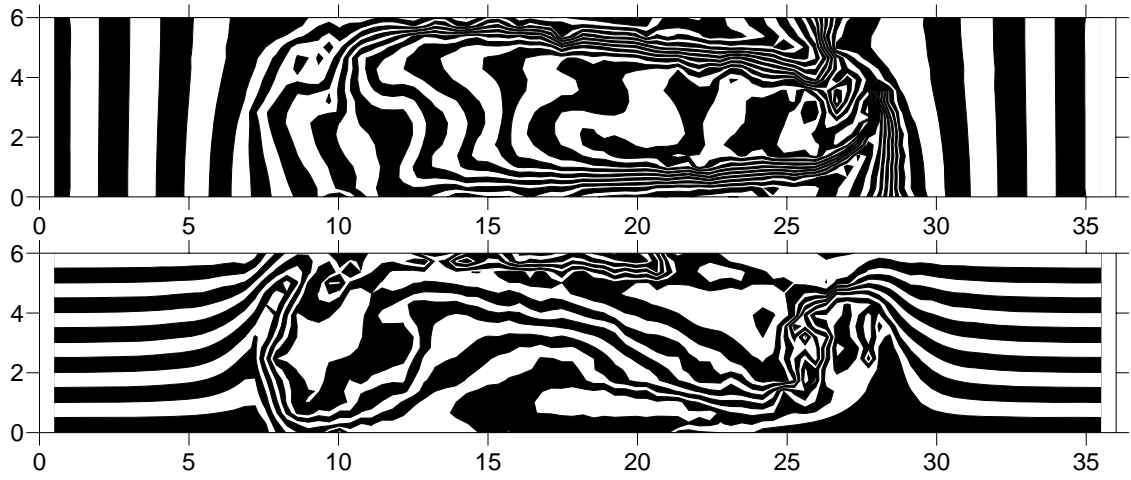


Fig. 5 Outflow streamtube pattern from vertical (above) and horizontal (below) inflow pattern for isotropic matrix with anisotropic single lens with $\kappa=\pi/4$ and $\psi=-0.332$.

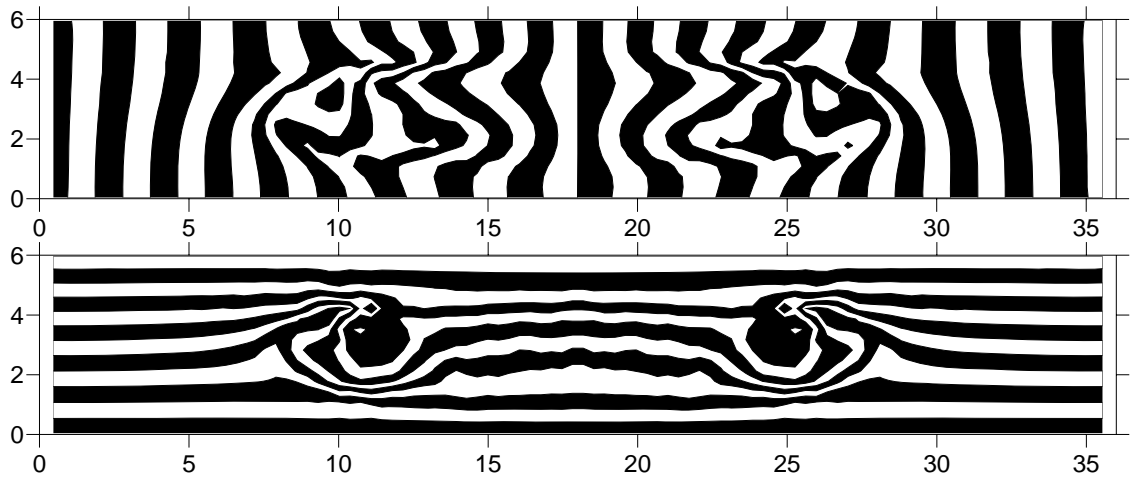


Fig. 6 Outflow streamtube pattern from vertical (above) and horizontal (below) inflow pattern for anisotropic matrix with anisotropic single lens with $\kappa=0$ and $\psi=-0.332$.

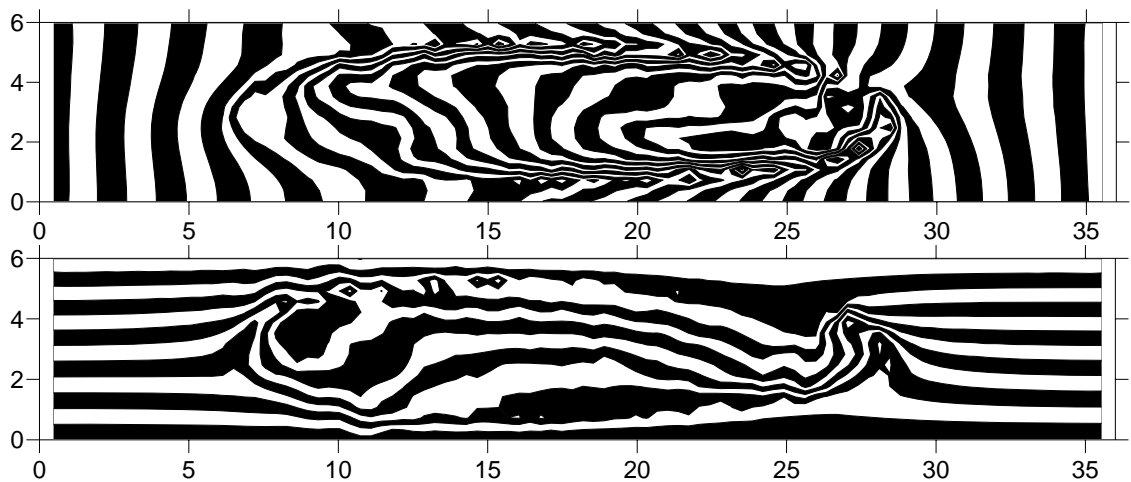


Fig. 7 Outflow streamtube pattern from vertical (above) and horizontal (below) inflow pattern for anisotropic matrix with anisotropic single lens with $\kappa=\pi/4$ and $\psi=-0.332$.

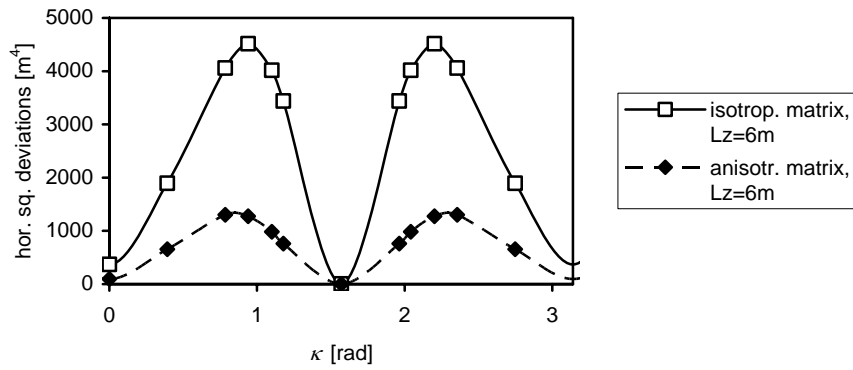


Fig. 8 Weighted squared horizontal deviations as function of horizontal angle κ of the principal direction of the hydraulic conductivity tensor of the lens.

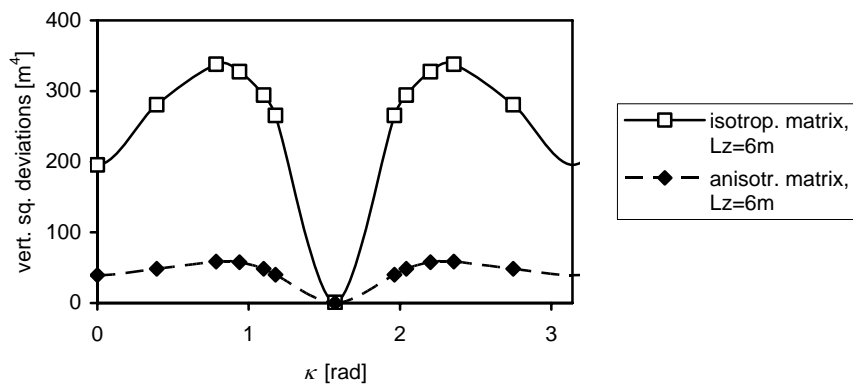


Fig. 9 Weighted squared vertical deviations as function of horizontal angle κ of the principal direction of the hydraulic conductivity tensor of the lens.

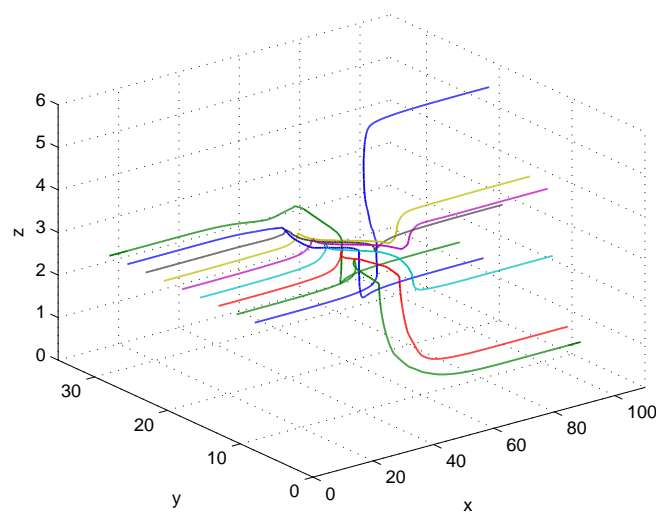


Fig. 10 Selected particle tracks for isotropic matrix with anisotropic single lens with $\kappa=\pi/4$ and $\psi=-0.332$.

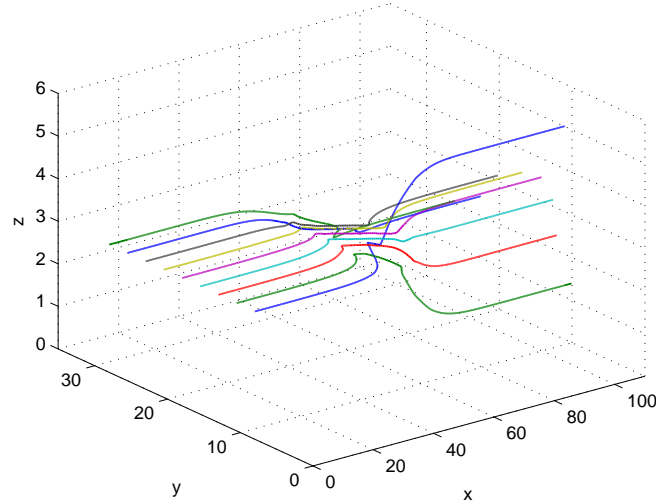


Fig. 11 Selected particle tracks for anisotropic matrix with anisotropic single lens with $\kappa=\pi/4$ and $\psi=-0.332$.

DISCUSSION AND CONCLUSIONS

The investigated flow domain corresponds to a shallow aquifer. Without additional highly conductive single inclusion lens it represents an aquifer with mean uniform flow. The single lens inclusion is relatively small and represents in our case a fraction of only 0.0084 of the total volume or 0.046 of the cross section. The effect of this single lens on the flow field very much depends on the anisotropy parameters of the lens. Anisotropic lenses with inclined principal direction of the hydraulic conductivity tensor show a strong impact on the flow field. On the other hand, isotropic lenses, or anisotropic lenses with inclination $\psi=0$, or anisotropic lenses with horizontal direction angle $\kappa=\pm\pi/2$ (with respect to the x -axis) show no or practically no disturbance of the flow field, provided the distance between the single lens and the outflow face is large enough. The distortion effect can be demonstrated by visualizing streamtube patterns consisting of vertical and horizontal stripes in the inflow face. The effect very much depends on the angle κ and the inclination ψ . The maximum effect was observed for a horizontal angle of about $\kappa=\pm 0.9$. The disturbance manifests itself by a distinct distortion of the streamtubes (Fig. 4 and 5). Vertically, the whole aquifer thickness is strongly influenced (Fig. 4 to 7). It can be expected that for a much larger aquifer thickness the influence would decrease with increasing vertical distance from the lens. Horizontally, the influenced width is about 2.5 times the width of the lens for the considered case (Fig. 4 to 7). The distortion effect can also be characterized by considering the sum of the weighted squared vertical and horizontal deviations of the particles in the outflow face compared to the situation without lens (Fig. 8 and 9). The resulting pattern suggests a whirl-like or spiral-like movement of the advecting particles. The analysis of single particle tracks (Fig. 10 and 11) supports this behaviour to some degree. Moreover, the pattern is in some qualitative correspondence with the findings of Hemker et al. (2004) and Bakker and Hemker (2004). They found a pronounced spiral like flow behaviour of particle tracks in horizontally layered aquifer blocks with horizontal anisotropy. In our study we can show that pronounced distortion of the particle tracks and some spiral-like behaviour is present also in the case of a relatively small anisotropic highly permeable lens with inclined plane of maximum hydraulic conduc-

tivity, which is imbedded in a background matrix as observed in natural sandy gravel deposits. However, anisotropy of the surrounding gravel matrix itself has a clear dampening effect by considerably reducing the degree of disturbance of the flow field (Fig. 6 and 7). Such anisotropy is often present as the results of a diffuse more or less horizontal layering or bedding. The chosen ratio of $K_{hor}/K_{vert}=10$ is typical for the sandy gravel formations under investigation. Still a well pronounced disturbance effect is present also in the anisotropic case. It can be expected that the effect of highly conductive single anisotropic lenses on solute transport may be considerable and may manifest itself by increased macrodispersivity values. The phenomena as presented in this study using a single lens configuration in a block-shaped aquifer matrix can better explain the numerical results of the stochastic facies modelling of Stauffer and Rauber (1998) in a qualitative manner. The results enable an improved understanding of the disordering advective processes, which may induce increased macrodispersion effects in heterogeneous gravel aquifers at the local scale.

REFERENCES

- Bakker M., Hemker K. (2004) Analytic solutions for groundwater whirls in box-shaped, layered anisotropic aquifers. *Advances in Water Resources* **27**, 1075-1086.
- Dagan G. (1989) Time-dependent macrodispersion for solute transport in anisotropic heterogeneous aquifers. *Water Resources Research* **24**(9) 1491-1500.
- Hemker K., van den Berg E., Bakker M. (2004) Ground water whirls. *Ground Water* **42**(2) 234-242.
- Jussel P., Stauffer F., Dracos T. (1994) Transport modeling in heterogeneous aquifers: 1. Statistical description and numerical generation of gravel deposits. *Water Resources Research* **30**(8) 1803-1817.
- Jussel P., Stauffer F., Dracos T. (1994) Transport modeling in heterogeneous aquifers: 2. Three-dimensional transport model and stochastic numerical tracer experiments. *Water Resources Research* **30**(8) 1819-1831.
- Stauffer F., Rauber M. (1998) Stochastic macrodispersion models for gravel aquifers. *Journal of Hydraulic Research* **36**(6) 885-896.