Characterization of Quaternary gravel aquifers and their implementation in hydrogeological models

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Abstract Aquifer analogues of Quaternary gravel deposits at two research sites in SW Germany were assembled. Detailed 2-D and 3-D sedimentological models were developed in the mesoscale (tens of metres) from sedimentological, hydrogeological, and geophysical surveys. Data from field investigations were integrated in facies models using ArcInfo GIS and GoCAD, respectively, delineating sedimentary structures and providing a database for hydraulic properties. A method was developed to convert these data into groundwater flow models using MODFLOW 2000 and related software. These were utilized to obtain bulk hydraulic flow and transport properties of the investigated sites.

Key words aquifer analogue; heterogeneity; gravel deposit; GoCAD; MODFLOW 2000; transport characteristics

INTRODUCTION

Gravel aquifers represent a major resource of drinking water. A general problem, however, exists in the characterization of sedimentary heterogeneities that affect groundwater flow as well as the transport of solutes and contaminants. The aquifer analogue approach is promising for study of sedimentary heterogeneity and to improve the predicting capabilities of hydrogeological modelling (Whittaker & Teutsch, 1999; Heinz et al., 2003).

In this study, results from field investigations including geophysical, sedimentological and hydrogeological methods, were integrated into detailed aquifer analogue models that could be used to realistically simulate groundwater flow and solute transport within the scale of investigation. Automated data conversion from sedimentological models using GoCAD or GIS is very useful for implementing large 3-D datasets or a number of different realizations in groundwater flow models such as MODFLOW 2000 (MF2k). A data conversion scheme suitable for that purpose was designed.

Approaches to upscale flow and transport characteristics need to rely on representative values of hydraulic properties. Hydrogeological simulations based on sedimentological models from integrated medium- to large-scale field investigations can help to provide such representative groundwater flow and transport characteristics of larger sedimentological facies units.
MODEL IMPLEMENTATION

GoCAD is a commercial application, specialized in the construction of surfaces, the
analysis of spatially distributed data and the modelling of properties. MODFLOW
2000 (MF2k, Harbaugh et al., 2000) is a widely used public domain code for the
simulation of groundwater flow processes. A method was developed to convert spatial
distribution data created by GoCAD, like 3-D distributions of hydraulic conductivity
$K$, directly into MODFLOW compatible input data, based on the automated file input
routine Teo3D (Bürger, 2004).

The GoCAD to MODFLOW model and data conversion proceeds in three steps. In
the first step, coordinate data in GoCAD format “cell centred” or “corner centred” are
transformed to a binary matrix that can be read by Teo3D. In the second step, the
MODFLOW 2000 (MF2k) input files are created using TEO3D (Bürger, 2003). After
that, the running of groundwater flow and transport models like MF2k (hydraulic flow
model) MPATH (particle tracking transport model), or the optional use of additional
models, completes the procedure.

The input data structure for MODFLOW is generated from a generic simple model
with uniform values of hydraulic conductivity $K$, porosity $n$, grid spacing ($\Delta x, \Delta y, \Delta z$),
boundary and initial conditions. Additional input of a generic heterogeneous model
requires the cell by cell specification of heterogeneous arrays of $K$, $n$, vertical grid
spacing $\Delta z$ (layer bottom and top elevation), boundary conditions, initial condition
(starting heads) and pumping wells. User defined data manipulation and vertical grid
refinement can be supplemented. In a similar way, the 2-D spatial distribution of
subsurface properties can be converted to a matrix format from ArcView/ArcInfo GIS
and loaded into MODFLOW.

DETERMINATION OF FLOW AND TRANSPORT PARAMETERS

Hydraulic conductivity ($K$) values representative for the model domain were obtained
by applying a gradient between constant head boundaries to the 3-D aquifer model in
the $x$, $y$ and $z$ directions, respectively, and extracting the resulting groundwater flow $Q$
from the model results. According to Darcy’s law, the bulk hydraulic conductivity
becomes $K_{bulk} = Q A^{-1} \ grad^{-1}$, where $A$ denotes the inflow area, and $\ grad$ the hydraulic
gradient.

Transport parameters can be determined using temporal moments of particle
breakthrough at certain locations (Cirpka & Kitanidis, 2000). Macroscale dispersion
characteristics can be obtained from breakthrough times integrated over the outflow
boundary, whereas temporal moments at discrete locations will yield information about
local scale effective dispersivities contributing to mixing of dissolved compounds.

The zero-th temporal moment is defined as:

$$m_0(x) = \int_0^\infty c(x,t)dt$$

(1)

The physical meaning of the zero-th temporal moment $m_0$ is the dissolved mass of
the given compound, or in a particle tracking simulation, the number of all particles
($np$) passing the location.
The first temporal moment is:

\[
m_1(x) = \int_0^\infty t \cdot c(x,t) dt
\]  

\(m_1/m_0\) represents the time of breakthrough of the mass centre at the given location. For particle tracking simulations, the first temporal moment equals the sum of the breakthrough times of all particles \(m_1 = \Sigma t\), and \(m_1/m_0\) is the arithmetic mean of the breakthrough times. The average groundwater flow velocity can be derived from the relationship \(m_1/m_0 = x/v\).

The second temporal moment, defined as:

\[
m_2(x) = \int_0^\infty t^2 \cdot c(x,t) dt
\]  

or the second centred temporal moment, respectively:

\[
m_{2c}(x) = \int_0^\infty (t - \frac{m_1(x)}{m_0(x)})^2 \cdot c(x,t) dt = m_2(x) - \frac{m_1^2(x)}{m_0(x)}
\]  

describes the deviation of transported mass from the centre of mass. \(m_{2c}/m_0\) in a particle tracking simulation equals the variance of the breakthrough times. From \(m_{2c}/m_0 = 2Dx/v^3\) follows the longitudinal dispersion coefficient. Local dispersion and molecular diffusion, however, cannot be accounted for using MODPATH; dispersion is only introduced into the flow system by spatial (and temporal) variations of advective flow.

If the rate of outflow at a certain location or the rate of pumping, respectively, is known, relative concentrations \(C/C_0\) can be calculated from the sorted breakthrough times of the particles:

\[
C/C_0 = \frac{\Delta t^{-1}}{QC_0}
\]  

where \(Q\) is the pumping or outflow rate (\(l s^{-1}\)) and \(\Delta t = t_i - t_{i-1}\) denotes the time difference between two particle breakthroughs within a given area. \(C_0\) is the total number of particles over the particle source volume. The so obtained breakthrough curve can be smoothed by averaging over a certain time interval.

**AQUIFER ANALOGUE STUDIES**

**Outcrop investigation**

The “Herten” gravel pit consists of structurally complex braided river deposits. During the excavation of the quarry wall, photographs of the fresh outcrop were taken and then digitized and built into an ArcInfo GIS as six parallel aquifer analogue cross sections (Bayer, 1999, Fig. 1).

In real aquifers no outcrop images are available, but geophysical methods (e.g. radar, seismics) can be utilised to delineate the spatial structure of the subsurface. In
the Herten site, images from ground penetrating radar (GPR, left) could be correlated well with the observed structures (Fig. 2). Based on images of the aquifer structure, maps of lithological units can be generated.

Hydraulic properties of lithofacies units from a large number of samples were determined by several authors and are representative of proglacial river deposits in southwest Germany (Heinz et al., 2003; Table 1). For \textit{in situ} conditions, empirical relationships from non-invasive survey techniques can be used to transform geophysical properties to hydraulic conductivity $K$ and porosity $n$ (Becht et al., 2004). From empirical relationships shown in Table 1, values of $K$ and $n$ were assigned to the underground structural elements (Bayer, 1999, Fig. 3).
Table 1 Representative hydraulic properties of gravel deposits in southwest Germany, obtained by grain size distributions and flowmeter measurements, from Heinz et al., (2003) and Kostic (2004).

<table>
<thead>
<tr>
<th>Lithofacies</th>
<th>Hydrofacies</th>
<th>Porosity (Heinz et al., 2003)</th>
<th>$K_f$ [m/s] measured (Flowmeter data)</th>
<th>$K_f$ [m/s] calculated</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gcg,a</td>
<td>cGcg,o</td>
<td>0.26 ± 0.02</td>
<td>$2.6 \times 10^{-2} \pm 2.3 \times 10^{-2}$</td>
<td>$2.4 \times 10^{-2} \pm 8.4 \times 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>Gcg,o</td>
<td>0.26 ± 0.02</td>
<td>$1.3 \times 10^{-3} \pm 7.4 \times 10^{-2}$</td>
<td>$2.8 \times 10^{-1} \pm 5.4 \times 10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>Gcm,b</td>
<td>0.2 ± 0.08</td>
<td>$7.4 \times 10^{-4} \pm 6.0 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>cGcm,b</td>
<td>0.2 ± 0.08</td>
<td>$5.0 \times 10^{-5} \pm 2.0 \times 10^{-4}$</td>
<td>$9.8 \times 10^{-5} \pm 8.6 \times 10^{-6}$</td>
</tr>
<tr>
<td>Gcx</td>
<td>cGcx</td>
<td>0.18 ± 0.03</td>
<td>$4.0 \times 10^{-2} \pm 2.8 \times 10^{-2}$</td>
<td>$1.0 \times 10^{-3} \pm 7.7 \times 10^{-4}$</td>
</tr>
<tr>
<td></td>
<td>Gcx</td>
<td>0.18 ± 0.03</td>
<td>$1.2 \times 10^{-3} \pm 9.3 \times 10^{-4}$</td>
<td>$7.5 \times 10^{-4} \pm 1.8 \times 10^{-4}$</td>
</tr>
<tr>
<td>Gmx</td>
<td>Gcx-Gmx</td>
<td>0.17 ± 0.07</td>
<td>$3.1 \times 10^{-3} \pm 1.2 \times 10^{-3}$</td>
<td>$2.9 \times 10^{-4} \pm 5.1 \times 10^{-5}$</td>
</tr>
<tr>
<td></td>
<td>Gmx</td>
<td>0.17 ± 0.07</td>
<td>$6.2 \times 10^{-4} \pm 3.2 \times 10^{-4}$</td>
<td>$2.5 \times 10^{-4} \pm 8.4 \times 10^{-5}$</td>
</tr>
<tr>
<td>GS-x</td>
<td>GS-x</td>
<td>0.27 ± 0.07</td>
<td>$2.1 \times 10^{-4} \pm 6.3 \times 10^{-5}$</td>
<td></td>
</tr>
<tr>
<td>S-x</td>
<td>S-x</td>
<td>0.36 ± 0.04</td>
<td>$1.0 \times 10^{-5} \pm 3.7 \times 10^{-5}$</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 3 Hydraulic conductivity distribution assigned to the lithological units in a vertical cross section of the Herten gravel pit, southwest Germany for the quarry wall shown in Fig. 1.

A steady state groundwater flow model was generated based on the given distribution of hydraulic conductivities, using MODFLOW 2000 (MF2k, see Fig. 4). Underlying the steady state head distribution of the flow model, particle tracking transport simulations using MODPATH were performed (Fig. 5). As indicated by the head distribution as well as particle pathlines from transport simulations, flow is concentrated in highly permeable channels to which the particles are attracted.

Bulk hydraulic flow and transport characteristics such as $K$ or longitudinal dispersivity ($\alpha_L$) of larger sedimentological units were obtained from the simulations. The results for the Herten gravel pit are:

$K$ [m s$^{-1}$]: 4.76e-04 (horizontal)

1.21e-04 (vertical)

$\alpha_L$ [m] 6.44

(horizontal)
Hydraulic head distribution of a steady state flow field simulated using MODFLOW, in a vertical cross section of the aquifer analogue model for Herten, southwest Germany corresponding to the outcrop image in Fig. 1.

Particle pathlines starting from the left boundary generated using MODPATH for the flow simulation in a vertical cross section shown in Fig. 4.

Integrated approach

At the Tettnang test site in southwest Germany, five boreholes were installed in the saturated zone of a gravel pit, down to a depth of 25 m. The area is formed by periglacial deltaic deposits containing very high permeable “open framework” gravel layers.

The site was investigated using an integrated approach involving sieve analyses, mapping and extrapolation of the surrounding outcrops, seismic and radar (GPR) borehole tomography as well as surface measurements, neutron and gamma logs, a short pumping test and flowmeter measurements (Kostic et al., 2003; Wagner, 2003; Becht et al., 2004). The spatial structure as well as quantitative properties could be delineated. Information gathered that way was compiled in a 3-D GoCAD facies model (Fig. 6). Dipping layers of different conductivity are visible in the 3-D block. The white layer represents a matrix free gravel (open framework) with extremely high conductivity.
GoCAD was used to create 25 equally probable realizations of $K$-distribution, conditioned on sieve analyses and flowmeter measurements in the boreholes. The so created 3-D K-field was implemented in a groundwater flow model using MODFLOW 2000. A deformed mesh (left) in vertical dimension was applied to optimize for layer-parallel flow.

A general problem exists in hydraulic testing of very high permeable aquifers. Only small drawdowns due to pumping were observed. Tracer movement, as indicated by the particle tracking simulation (Fig. 7), is likely to bypass the central pumping well in high conductivity channels (dark lines). A tracer experiment has only a poor chance of recovery if the tracer is injected into the layer of high conductivity or below, so tracer testing had to be omitted.

The flow model and particle tracking simulations using MODPATH were also used to obtain flow and transport characteristics (Table 2). Sets of cumulated particle
Fig. 7 Steady state flow and particle tracking simulation for a pumping test at a central well, Tettnang test site gravel pit, southwest Germany. Particle pathlines for a tracer injected at the zone of high conductivity are marked in white.

Table 2 Anisotropy of bulk hydraulic conductivity for flow simulations of the Tettnang test site.

<table>
<thead>
<tr>
<th></th>
<th>Mean $K$ (m s$^{-1}$)</th>
<th>$K$ standard deviation (m s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X$</td>
<td>7.053E-03</td>
<td>3.043E-04</td>
</tr>
<tr>
<td>$Y$</td>
<td>1.069E-02</td>
<td>4.047E-04</td>
</tr>
<tr>
<td>$Z$</td>
<td>1.814E-03</td>
<td>1.287E-04</td>
</tr>
</tbody>
</table>

breakthrough curves differ remarkably between zones of different conductivity and provide a base to estimate dispersivity. In Fig. 8 an example of a simulated breakthrough curve at the pumping location is shown. In this case, the particles are injected at a depth of 6 m, above the zone of high permeability, resulting in more than 90% recovery.

Temporal moment calculations yielded a bulk longitudinal dispersivity ($\alpha_L$) at the mesoscale of the highly resolved 3-D block of 13 m. Dispersivity values, however, also depend on the scale of investigation and require further research. Representative values may be expected from investigations that encompass complete sedimentological settings, i.e. the whole delta complex in the given case.
CONCLUSIONS

Data from detailed field investigations, so called aquifer-analogue studies, at two sites in southwest Germany were converted to high resolution 2-D and 3-D hydrogeological models. Flow and transport characteristics for this scale of investigation could be delineated. However, due to difficulties in hydraulic testing in extremely permeable geological materials, the results could not be compared to field measurements such as tracer tests. More representative aquifer properties of typical sedimentological deposition facies can be expected from a greater number of investigations and larger scales. Hydraulic flow and transport characteristics obtained from aquifer analogue studies can help to improve management of groundwater resources and contribute to groundwater risk assessment for point or diffuse sources of contamination and their natural attenuation perspectives.

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REFERENCES


