Estimation of contaminant mass flows in a multi-layered aquifer using pumping tests: numerical experiments at field-scale

M. Bayer-Raich, R. Baumann & T. Ptak
Center for Applied Geoscience, University of Tübingen, Sigwartstrasse 10, D-72076 Tübingen, Germany

Abstract Analytical solutions to the integral groundwater investigation approach (Teutsch et al., 2000) based on pumping tests were applied in numerical experiments at the field scale in a multi-layered aquifer system to quantify the mass flow of contaminants in groundwater. Both a depth integrating and a new multi-layered set-up were used to derive layer-oriented information about the mass flows. For the scenario investigated, the depth integrating approach gives an acceptable estimation of the total mass flow over the whole aquifer thickness. However, to get vertically differentiated information on the contamination it is necessary to apply the multi-layered approach which yields reasonable results despite some simplifying assumptions.

Key words analytical inversion; Bitterfeld, Germany; field scale; integral groundwater investigation approach; mass flow; multi-layered aquifer; pumping test; SAFIRA; transport model

INTRODUCTION

An integral groundwater investigation approach to estimate total contaminant mass flows using pumping tests was proposed in Teutsch et al. (2000) and applied by Ptak et al. (2000) and Bockelmann et al. (2001) at the field scale under natural groundwater flow conditions. The objective is to obtain a more precise assessment of the groundwater contamination at field scale, compared to conventional point-scale concentration measurements. First numerical simulations in a (moderately) heterogeneous synthetic example performed by Bayer-Raich et al. (2001) showed that the method provides good estimates of the total contaminant mass flow. The basic idea of the integral approach is to increase the sampled volume of water through pumping tests, during which the natural flow conditions are temporarily changed and the contaminant concentration in the pumping well as a function of time \(t\), \(c(t)\), is measured. The sampled concentrations in this time series represent average concentrations along isochrones, which can be described as circles of radius \(r(t)\) when the background natural flow is small compared to the radial flow towards the well (otherwise the isochrones have to be described as \(r(Q,t)\)). Using these average isochrone concentrations and calculated isochrone positions as a function of time, we can analytically estimate the average plume concentration at a control plane perpendicular to the groundwater flow direction as a function of the radial distance to the well centre, \(c(r(t))\), before the start of the pumping test. To estimate the resulting mass flow \(M\) of contaminants across the control plane under natural flow conditions, Schwarz (2001) developed an analytical solution (see below) on the basis of \(c(r(t))\), information
on hydraulic conductivity and the natural hydraulic gradient. The solution is based on the following two main assumptions: (a) contaminant concentration is constant along a streamtube at the length scale of the captured zone in the pumping test, and (b) there is no significant instantaneous sorption as the plume is moved during pumping.

In this paper, we use the integral investigation approach described above to analyse a numerical realization of a contaminant plume in a heterogeneous, multi-layered aquifer, relevant for field-scale conditions. In the numerical realization, or experiment, using a real site model we first generate numerically a contaminant plume originating from a source zone which is situated over three layers in a fully three-dimensional simulation domain. We then obtain input data for the integral investigation approach by performing numerical pumping tests, in which we observe the contaminant concentration \( c \) in the pumping well as a function of time \( t \). Based on the observed \( c(t) \)-curves, the integral investigation approach is used to estimate plume position and concentration, and mass flow \( M \) under natural flow conditions, considering two different methods: (I) the application of a depth-integrated version where we do not consider the aquifer as being multi-layered with different hydrogeological properties; (II) the application of a new multi-layered version where we consider the aquifer as multi-layered, as often observed under natural conditions. Finally, we compare the results to the actual values for the total contaminant mass flows over all layers (methods I and II) and separately for each layer (method II) to assess the estimated quality of the results referring to the plume position and total emitted mass flow.

FIELD SITE, GROUNDWATER MODEL AND NUMERICAL EXPERIMENTS

A field site is available for application at Bitterfeld (Sachsen-Anhalt, Germany). It has been investigated for many years within the framework of an interdisciplinary project called SAFIRA (Sanierungsforschung In Regional kontaminierten Aquiferen). The hydrogeological situation of this field site is documented in Böhme & Falke (1999).

Field site The investigation area includes the southern part of the “Chemiepark Bitterfeld” and covers an area of nearly 2.5 km\(^2\). The upper part of the aquifer (called aquifer 110) is composed of Quaternary sediments (sand and gravel) with different local facies. Directly below this aquifer is the Tertiary aquifer 500 (also called Bitterfelder Glimmersande) which mainly consists of finer sand formations in comparison to aquifer 110. The base of the complete aquifer system consists of clay and silt formations (called Gaukonitschluff and Rupelton). In general there is a hydraulic connection and a hydrogeochemical similarity between the two aquifers. The hydraulic gradient is of the order of 0.1%, and the groundwater flow direction is oriented west–east in both aquifers. Due to the generally lower hydraulic conductivities in aquifer 500 the groundwater velocities are in the range of two orders of magnitude lower than the average velocity in aquifer 110. Using flow meter measurements in aquifer 110 it was shown that hydraulic conductivity varies by nearly three orders of magnitude in the vertical direction, with a mean hydraulic conductivity of \( 4.2 \times 10^{-4} \) m s\(^{-1}\). In addition, a multilevel observation well was installed, and measurements in 12 different aquifer levels were carried out. Contamination (especially by benzene/monochlorobenzene) was observed over the whole vertical profile at concen-
trations between 1 and more than 10 mg l\(^{-1}\). The highest contaminant concentration level was at the bottom of aquifer 110 and in the upper part of aquifer 500.

**Groundwater flow and transport model** In the framework of the SAFIRA project a regional groundwater flow and transport model was developed by Borkert (1999) for transient flow conditions. The application of the integral investigation approach was carried out employing an adapted version of this transient groundwater flow and transport model.

The model was created using the graphical interface Visual MODFLOW for the numerical program code MODFLOW (McDonald & Harbaugh, 1988). The model area is located between the Gauss-Krüger coordinates 4519000 and 4525000 (west–east direction) and 5724000 and 5717500 (north–south direction) and covers 39 km\(^2\). The model grid is discretized by cell widths of between 25 and 200 m. At the pumping well locations, a grid refinement down to 0.5 m was introduced. The aquifer thickness of about 45 m is represented by eight layers. Layer 1 corresponds to an artificial fill, layers 2 to 4 represent the Quaternary aquifer 110, and layers 5 to 8 the Tertiary aquifer 500 in the vicinity of the test site. The mean groundwater recharge amounts to about 3.11 s\(^{-1}\) km\(^{-2}\). The detailed distribution of the hydraulic parameters and the boundary conditions are documented in Borkert (1999).

**Numerical experiments** The first step in the numerical experiments was the generation of a plume. Therefore we introduced a contaminant source with a length (north–south direction) of 30 m and a width (east–west direction) of 5 m into the model domain. The source was placed in layers 2, 3 and 4, with different fixed contaminant concentrations. Concentrations of 0.5 mg l\(^{-1}\) in layer 2, 0.1 mg l\(^{-1}\) in layer 3 and 1 mg l\(^{-1}\) in layer 4 were used. The distance from the source to the pumping well was about 160 m. For the generation of the plume a transient simulation over a time period of 10 years was performed. During this simulation the contaminant source acted as a constant concentration boundary condition. The second step dealt with simulating the pumping test employed in the integral investigation approach. For this pumping test a well location outside the generated plume was selected (see Figs 1 and 2). The well was represented by a column of model cells with high hydraulic conductivity. A constant pumping rate of 10 l s\(^{-1}\) and a pumping time of 14 days were chosen. Two different numerical experiments where carried out. In the depth-integrated experiment I, 10 “samples” (c(t)-values) of the groundwater pumped at the well were collected at the “pump inlet” (model cell where discharge is applied), i.e. only one depth-integrated c(t)-curve was generated. In the multi-layered numerical experiment, II, 8 samples were taken from layer 2, another 8 samples from layer 3, and 10 from layer 4. In the field, a new multilevel sampling technique allowing multilevel groundwater samples to be obtained from pumped wells will be applied with measurements at the SAFIRA site.

**APPLICATION OF THE DEPTH-INTEGRATED INTEGRAL INVESTIGATION APPROACH**

When there is no information about the multi-layered nature of an aquifer, it is common to assume homogeneous conditions. In this section we apply the depth-integrated approach using the c(t)-curve arising from numerical experiment I in an
equivalent homogeneous aquifer. The aquifer is characterized by a constant estimate of the effective value for porosity, hydraulic conductivity and saturated thickness.

For the inversion, the following analytical equation is used (Schwarz, 2001):

\[
M = 2 \sum_{i=1}^{n} c_i Q_i \quad \text{with} \quad c_i = \frac{\pi}{2} - \sum_{k=1}^{i-1} \left( \frac{\arccos \left( \frac{r_{k+1}}{r_i} \right)}{\arccos \left( \frac{r_k}{r_i} \right)} - \frac{\arccos \left( \frac{r_{k-1}}{r_i} \right)}{\arccos \left( \frac{r_k}{r_i} \right)} \right) \quad (1)
\]

where \( M \) is mass flow perpendicular to the control plane, \( c_i \) representing the concentration measured at the pumping well at time \( t_i \), i.e. \( c(t_i) \), \( \hat{c}_i \) the average of the concentrations of the two streamtubes of the natural groundwater flow field positioned left and right from the pumping well at a distance \( r \) (with \( r_{i-1} < r < r_i \)). Note that \( Q_i = k_i \sqrt{h_i b_i} / \pi \phi_i \) is the natural flow rate perpendicular to the control plane at both left and right streamtubes and \( r_i = \sqrt{Q_i / \pi \phi_i} \) is the radius of the isochrone corresponding to \( t_i \) with \( Q \) the pumping rate at the well, \( b \) the aquifer thickness and \( \phi \) the porosity. For the first time step, \( \hat{c}_1 = c_1 \) and \( r_0 = 0 \), \( n \) is the total number of samples (a more detailed description can be found in Bockelmann et al. (2001)).

Figure 1(a) summarizes the upscaled values used for the characterization of the aquifer (considering a constant aquifer thickness of 11 m). The position of the plume when the pumping test started is shown in Fig. 2(b), where a steady-state mass flow of \( M = 8.8 \) g day\(^{-1}\) is crossing the control plane. As a result of the (numerical) pumping test described in the previous section the depth-integrated \( c(t) \)-curve shown in Fig. 1(c) is obtained. Both the method of characteristics (MOC) and finite differences (FD) were used in the numerical experiment. The 10 \( c(t) \)-values used for the inversion are shown in Fig. 1(c) as dots (estimates between the numerically generated \( c(t) \)-curves). The result of the inversion, i.e. the concentration distribution along the control plane, is shown in Fig. 1(d) in comparison with the concentration along the cross-section of the depth-integrated actual plume. The estimated mass flux arising from (1) equals \( M = 12.1 \) g day\(^{-1}\).

APPLICATION OF THE NEW MULTI-LAYERED INTEGRAL INVESTIGATION APPROACH

The main limitation of the depth-integrated approach, when considering stratified aquifers, is that it cannot indicate at which aquifer level the contamination is situated. In this section, we present a new multi-layered approach that overcomes this limitation. To account for the multi-layered nature of the aquifer, the total thickness of 11 m was divided into three homogeneous layers, as shown in Table 1. Different capture zones and pumping rates are considered in each layer to perform independent inversions in each layer.

Figure 2(a) shows the position of the plume in each layer (before the pumping starts), with steady-state mass flows of \( M_{L1} = 0.3 \) g day\(^{-1}\); \( M_{L2} = 0.6 \) g day\(^{-1}\) and \( M_{L3} = 7.5 \) g day\(^{-1}\), observed at the control plane. The \( c(t) \)-curves, Fig. 2(b), obtained from numerical experiment II (independent sampling in each layer employing both the MOC
Estimation of contaminant mass flows in a multi-layered aquifer using pumping tests

\[ T(x,y) = \int_{z_{\text{bottom}}}^{z_{\text{top}}} K(x,y,z) \, dz = 7.5 \times 10^{-3} \, \text{m}^3 \, \text{s}^{-1} \]

\[ \varphi(x,y) = \frac{1}{b} \int_{z_{\text{bottom}}}^{z_{\text{top}}} \varphi(x,y,z) \, dz = 0.22 \]

Fig. 1 Application of the depth-integrated integral investigation approach. (a) Characteristic aquifer parameters. (b) Two-dimensional plume and position of the control plane. (c) Depth-integrated \(c(t)\)-curve arising from the pumping test. (d) Estimated and actual values of concentration along the control plane.

<table>
<thead>
<tr>
<th>Layer</th>
<th>(K) (m s(^{-1}))</th>
<th>(b) (m)</th>
<th>(Q) (L s(^{-1}))</th>
<th>(r_{\text{max}}) (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layer 2</td>
<td>(0.5 \times 10^{-3})</td>
<td>0.2</td>
<td>4</td>
<td>2.5</td>
</tr>
<tr>
<td>Layer 3</td>
<td>(0.5 \times 10^{-3})</td>
<td>0.2</td>
<td>3</td>
<td>1.5</td>
</tr>
<tr>
<td>Layer 4</td>
<td>(10^{-4})</td>
<td>0.25</td>
<td>4</td>
<td>6</td>
</tr>
</tbody>
</table>

and FD methods) are inverted with (1), yielding the estimated concentrations (Fig. 2(c)) and the mass flows in the individual layers: \(M'_{L2} = 0.9\) g day\(^{-1}\); \(M'_{L3} = 1.6\) g day\(^{-1}\) and \(M'_{L4} = 10.3\) g day\(^{-1}\).

**CONCLUSIONS**

In this contribution we tested both the depth-integrated and the multi-layered versions of the integral investigation approach employing a contaminant plume generated in a three-dimensional advective transport model. The simulation time was 10 years with a constant emission of the contaminant. The mass flux was estimated at a control plane (located 160 m downstream of the source) through a (numerical) pumping test with both the depth-integrated (method I) and the new multi-layered (method II) integral investigation approaches. Figure 3 summarizes the mass flux estimates arising from both methods.
Both the depth-integrated and multi-layered approaches lead to good results. The overestimation in mass flows observed in Fig. 3 can be attributed to overestimation of the transmissivity in the layers and to vertical mixing during the pumping test.

The numerical experiment shows that it is possible to estimate the contaminant mass flow in each layer. The multi-layered approach is applicable in real aquifers when the (geological) layers are practically continuous within a zone around the pumping well, being large enough to avoid significant vertical gradients in the vicinity of the pumping well. The depth-integrated approach has already been applied in practice at several sites (e.g. Holder et al. (1998), Ptak et al. (2000), Bockelmann et al. (2001)). The new multi-layered version of the integral investigation approach will be applied for the first time under field conditions in Bitterfeld, using a new multilevel sampling technique allowing to obtain multilevel \( c(t) \)-curves during pumping.
REFERENCES


