Assessing contaminant mass flow rates obtained by the integral groundwater investigation method by using the Virtual Aquifer approach

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Abstract Contaminant mass flow rates originating from a contaminant source zone provide a basis for quantifying the environmental impact and may thus play an important role in assessing natural attenuation as a remedial or management option for contaminated aquifer cleanup. A reliable quantification of the contaminant mass flow rate is thus sought. The integral groundwater investigation method provides a possibility for estimating mass flow rates by using long-term pumping tests. This work focuses on the performance and reliability of this method in heterogeneous aquifers and under "realistic" conditions, representative of a typical site investigation. The Virtual Aquifer method is used for study. The results show that the method is mainly influenced by the hydraulic flow regime near the control plane, where uncertainty in hydraulic conductivity or estimated hydraulic gradient may severely influence the mass flow rate obtained. Determination of the average concentration along the control plane is much less uncertain.

Keywords integral groundwater investigation method; mass flow rates; monitoring strategy; uncertainty assessment

INTRODUCTION

The principal idea of the *virtual aquifer* is to simulate and evaluate contaminated site investigation strategies by using typical contamination scenarios (Schäfer *et al.*, 2002; Schäfer *et al.*, 2004; Bauer *et al.*, 2005; 2006). To achieve this goal, *typical aquifers*, closely related to reality, are generated in the computer and are polluted with a defined contaminant source. A transport model incorporating the processes governing the pollutant fate in the subsurface is then used to simulate the development of the contaminant plume within the virtual aquifer. The plume generated is then investigated, e.g. by using monitoring wells, just as in reality. However, in contrast to a real contaminated site, the "true" concentration distribution is known. By comparing the "measured" to the known "true" concentrations or other investigation results, the investigation strategy employed can be assessed and maybe improved.

The integral groundwater investigation method (compare Fig. 1), or integral pumping test method, is used here to quantify contaminant mass flow rates. The methodology has so far been applied at a number of study sites to estimate contaminant mass flow rates (Holder *et al.*, 1998; Bockelmann *et al.*, 2001; Bauer *et al.*, 2004), a study site based uncertainty investigation has been conducted by Jarsjö *et al.* (2003) and new theoretical developments are given in Bayer-Raich *et al.* (2004). In this approach, pumping wells positioned along control planes perpendicular to the

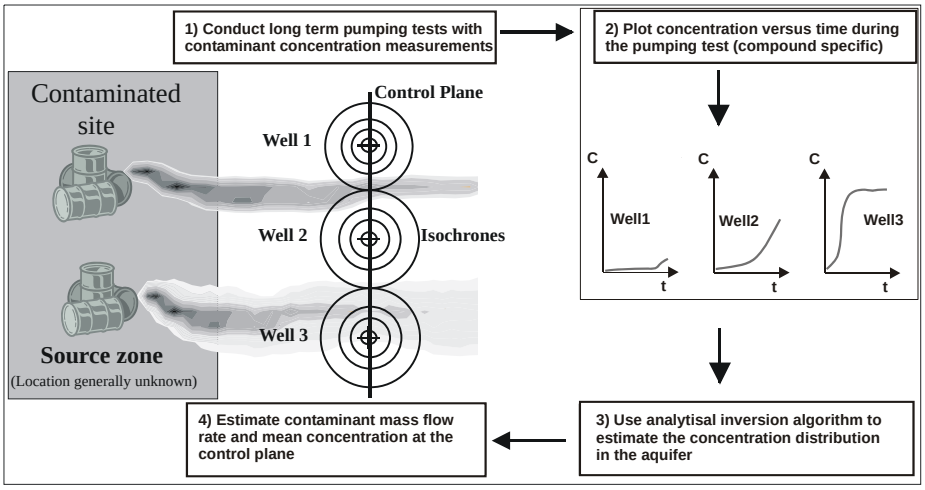

Fig. 1 Schematic representation of the integral groundwater investigation method Reprinted from Bauer *et al.* (2004) with permission from Elsevier, ©2004 Elsevier.

groundwater flow direction are operated for a time period on the order of a few days and sampled for contaminants in the pump discharge (Fig. 1). The concentration time series of the contaminants thus measured during operation of the pumping wells are then used to determine contaminant mass flow rates, mean concentrations and the plume shapes and positions at the control planes. This is performed by employing an analytical inversion methodology.

In this work, the determination of mass flow rates by the integral groundwater investigation method is studied by using the Virtual Aquifer approach. A virtual reality is generated by simulating the spreading of a plume originating from a defined source in a heterogeneous aquifer. This plume is investigated using monitoring wells, and from these the location for a control plane for mass flow rate or concentration determination is obtained. Integral pumping tests are then virtually conducted along the control plane and the "measurements" during the pumping test, i.e. drawdown and the contaminant concentration time series, are evaluated to yield contaminant mass flow rates and average contaminant concentrations at the control plane. These values are then compared to the "true" concentration distribution and the "true" mass flow rate.

METHODS

First, two-dimensional aquifers of 184 m length and 64 m width are generated, which are discretized by 0.5 × 0.5 m elements (Fig. 2(a)). Groundwater flows from left to right, driven by a hydraulic gradient of 0.003, induced by fixed head boundary conditions along the left and right hand side. The hydraulic conductivity is log-normally distributed with a mean of $\ln(K) = -9.54$, corresponding to 7.2×10^{-5} m s^{-1}. The spatial distribution of the hydraulic conductivity is described by an isotropic exponential covariance model, using an integral scale of 2.67 m and a variance σ^2_Y of 1.71. The value for the integral scale stems from the Borden field site (Sudicky, 1986), the variance was determined for a Quaternary alluvial aquifer in southern Germany (Herfort, 2000). At a distance 11.5 m downstream of the upstream model boundary, a

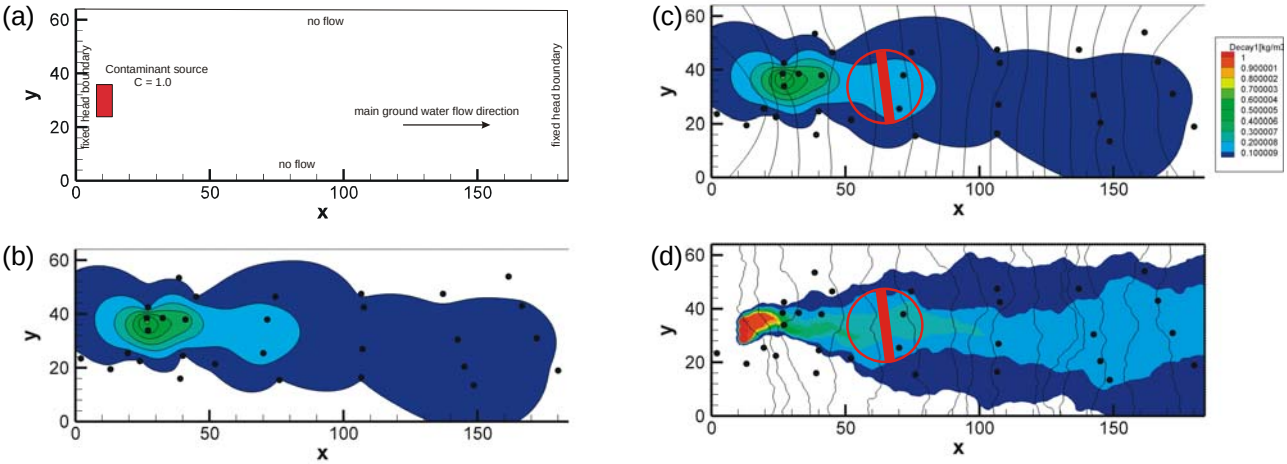

Fig. 2 Schematic representation of the Virtual Investigation by Integral Pumping Test. a) Model setup and boundary conditions, b) Plume investigated by observation wells and interpolation, c) location and design of the integral pumping test in the investigated plume, and d) integral pumping test in the "real" plume.

contaminant source is emplaced, emitting a non-reactive contaminant with source concentration 1.0. Source width is between 4 and 12 m. Porosity is 0.33, local longitudinal and transverse dispersivities are 0.5 m and 0.1 m. Thus the contaminant is transported with an average flow velocity of 6.5×10^{-7} m s^{-1}. The simulation code GeoSys (Kolditz & Bauer, 2004; Kolditz *et al.*, 2004), which is based on the standard Galerkin Finite Element Method, is used to calculate the steady-state plume evolution.

The evolved steady-state plume was investigated virtually using observation wells with a subsequent interpolation step, where the hydraulic heads and the concentrations found at the well locations were interpolated using kriging. The investigation steps: (a) placing new wells, and (b) interpolating the "measured" heads and concentrations were repeated, until the plume interpolation was found to be satisfactory (Fig. 2(b)). This plume interpolation was performed by a number of German scientists and hydrogeologists, and the task was to obtain a good plume investigation and interpolation by using any number of wells and interpolation steps. The results of the investigation are thus independent and yield individually and realistically investigated plumes.

The interpolation results are used as the basis for the investigation of the integral pumping test method (Fig. 2(c)). Based on the interpolated plume, a control plane is placed perpendicular to the main plume axis 50 m downstream of the contaminant source with a width of 20 m. Thus location and width of the control plane to be covered by integral pumping test for mass flow rate determination are defined. Other possibilities for locating the control plane would be depending on concentration, i.e. cover all of the plume with concentrations larger than 0.1 of the source concentration. For this investigation, just one pumping test was used. From the (known) aquifer porosity n, the aquifer thickness m of 10 m, the control plane width w and a pumping time t of 4.5 days the pumping rate Q needed to cover the given width can be calculated by:

$$Q = \pi m n w^2 t^{-1} \tag{1}$$

It is clear, that with increasing width of the control plane the pumping rate needed to achieve this width is increasing quadratically.

In the next step (Fig. 2(d), the pumping test is conducted. The pumping well is placed in the middle of the control plane with the corresponding pumping rate. To achieve valid numerical results, the finite element mesh is refined around the well, with element sizes close to the pumping well of 0.05 m rising to element sizes of 0.5 m at the control-plane ends. Small time steps of increasing size are used to simulate flow and transport in the evolving convergent flow field. In the pumping well, hydraulic heads and concentrations are recorded with time.

Evaluation of the pumping test starts by determination of the hydraulic conductivity (Fig. 3(a)). The "measured" drawdown data and the Cooper-Jacob method are used here to determine the hydraulic conductivity. In the second step (Fig. 3(b)), the analytical solution of the inversion problem (Schwartz *et al.*, 1998; Bayer-Raich *et al.*, 2004) is used to estimate mass flow rates across the control plane. This is a simplification, as this analytical solution assumes homogeneous aquifer properties and a negligible hydraulic gradient within the maximum isochrone developed. The analytical solution uses the aquifer thickness, the hydraulic conductivity (determined from the drawdown data), the hydraulic gradient across the control plane (determined from nearby wells of the interpolated plume), the porosity and the pumping rate to yield an estimate of the average concentration within the well capture zone as well as an estimate of the contaminant mass flow rate. Mass flow rate M and groundwater discharge across the control plane Q_{CP} as well as the average concentration in the well capture zone C_{Av} are related by:

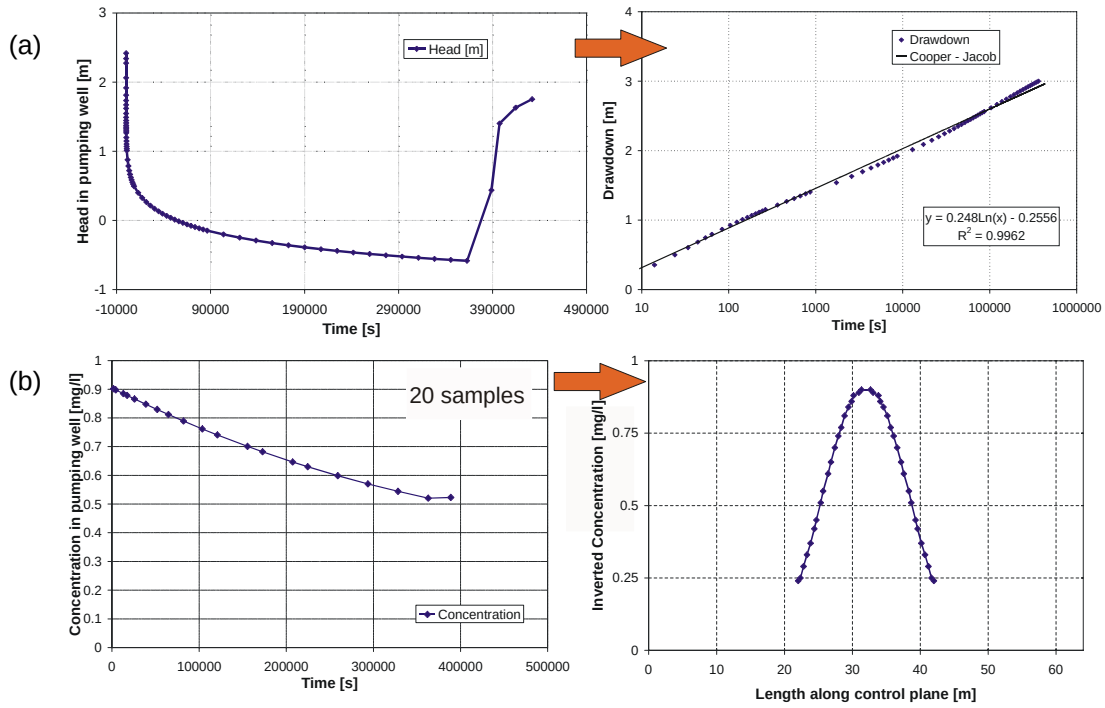

Fig. 3 Schematic representation of the Virtual Investigation by an Integral Pumping Test. (a) head observation in the pumping well (left) and drawdown data with fitted line for calculation of K by the Cooper-Jacob method; (b) observed concentration time series and inverted concentrations in aquifer along control plane.

$$M = Q_{CP} C_{Av} \tag{2}$$

The mass flow rate thus determined is compared to the true mass flow rate. The true mass flow rate is obtained from the results of the steady-state simulation prior to conducting the pumping test by adding up the local element mass flow rates along the control plane. This true mass flow rate thus accounts completely for the heterogeneity of the hydraulic conductivity. Additionally, the concentration distribution and the water flow rate along the control plane are calculated.

RESULTS AND DISCUSSION

Figure 4 summarizes the results of the assessment by the Virtual Aquifer approach of the integral groundwater investigation method. Shown are normalized values, i.e. the corresponding estimated parameter is normalized to the true value. For example, the normalized mass flow rate is the estimated mass flow rate divided by the true mass flow rate, and the better the estimate, the closer the shown value is to one (horizontal grey line). Figure 4 shows the results of the individual realizations as well as average values with standard deviations. As can be seen from Fig. 4, estimated mass flow rates deviate from the true mass flow rate. Mass flow rates may be overestimated by a factor of about 4 and underestimated by about a factor of 30. The same is true for the water flow rate, which shows a similar span of normalized values. Thus both mass flow rate and water flow rate show an uncertainty of more than one order of magnitude.

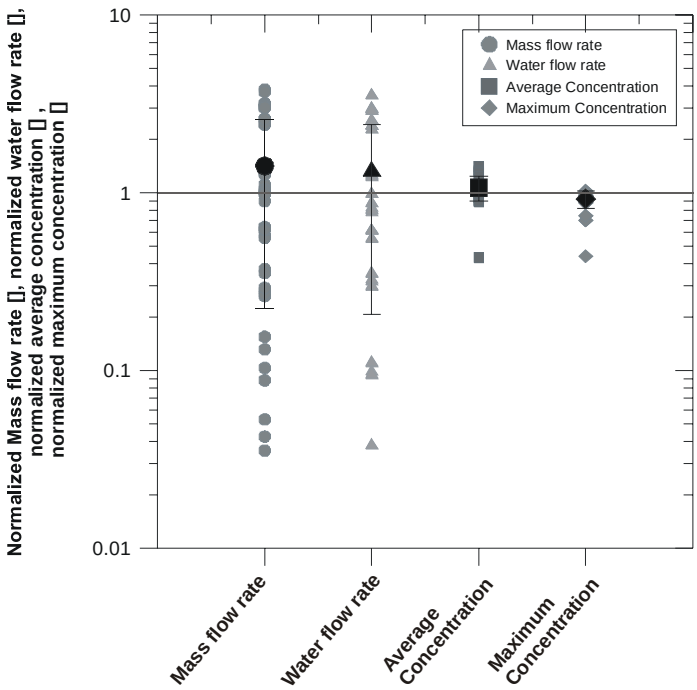

Fig. 4 Normalized results of the integral groundwater investigation, where values are normalized to their true values. The grey symbols denote the results from a single realization, the black symbols the arithmetic average and the error bars show one standard deviation.

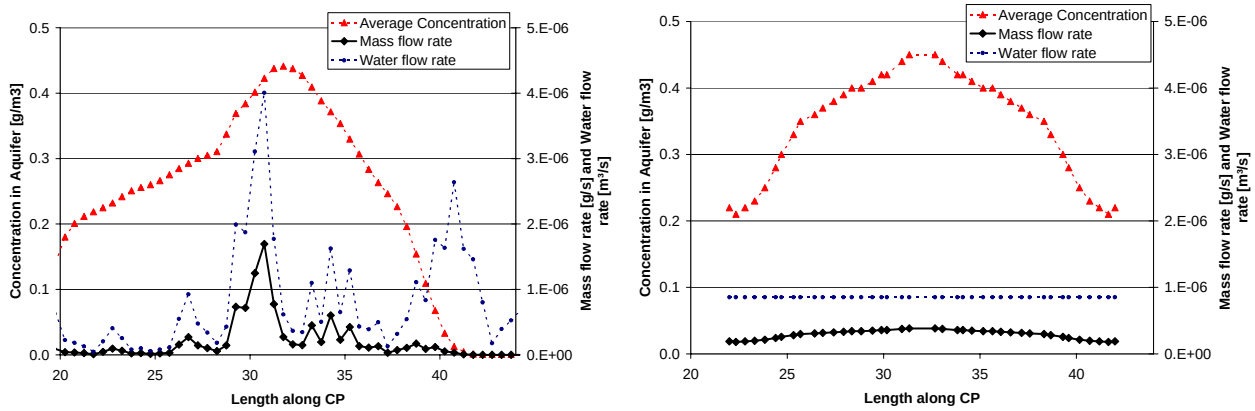

Fig. 5 Length profiles of concentration, mass flow rate and water flow rate along the control plane. Real values (left hand side) and values estimated by the inversion of pumping test data. The pumping well is positioned at 32 m, the control plane reaches from 22 to 42 m.

Determination of the average concentration is much more certain; the smallest estimated average concentration is 0.88, the largest 1.41. The maximum concentration within the largest isochrone during the pumping test is the parameter with the smallest uncertainty, the span ranges from 0.70 to 1.02. Mean and standard deviations for the mass flow rate, the water flow rate, the average concentration and the maximum concentration are 1.41 (±1.19), 1.31 (±1.11), 1.07 (±0. 17) and 0.92 (±0.11).

Figure 5 shows a typical result of the investigation. In this case, the correspondence between estimated and true parameters is good. The left hand side shows the real (although virtual) values of concentration in the aquifer, the mass flow rate and water flow rate along the control plane, while the right hand side shows the values estimated by the above described procedure. The real aquifer shows fluctuations in water flow rate across the control plane of about a factor of 10, causing also local fluctuations of the mass flow rate, which is given by the product of local water flow rate and local concentration. The estimated water flow rate is homogeneous along the control plane, yielding a smooth profile of the estimated mass flow rate. In the case of Fig. 5, the water flow rate is slightly underestimated, however the concentration is overestimated towards the ends of the control plane, causing in total a slight overestimation of the mass flow rate by 17%.

The estimated water flow rate is strongly influenced by the hydraulic conductivity determined by the long-term pumping test and the hydraulic gradient of the interpolated plume, as determined by the plume investigators. Both provide sources of error. As the correlation length of 8 m (corresponding to an integral scale of 2.66 m) is smaller than the size of the control plane by a factor of 2.5, the hydraulic conductivity determined from the pumping test may not be representative for the complete control plane. Both underestimation and overestimation of the hydraulic conductivity by up to a factor of 10 was found in this study. This directly causes an underestimation or overestimation of the mass flow rate of the same factor (compare equation (2)). The hydraulic gradient also linearly influences the mass flow rate, but here the uncertainty is lower and deviations found were smaller than a factor of 3.

Concerning the average concentration, overestimation occurs if the plume fringes are very sharp within the control plane. Underestimation occurs if the pumping well is

not positioned within the plume centre and contaminated water is pumped only at the end of the pumping test.

As is clear from Fig. 4, the dominating uncertainty is the uncertainty in water flow rate, stemming from uncertainty in determining the hydraulic conductivity and from uncertainty in interpolating the local hydraulic gradient across the control plane. In field applications, therefore, care should be taken to obtain a realistic representation of the hydraulic flow regime at and near the control plane. One of the possibilities would be to use multiple pumping tests along the control plane, thus yielding a better estimation of the hydraulic conductivity.

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