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Stochastic evaluation of mass discharge from pointlike concentration measurements

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ABSTRACT

The contaminant mass discharge crossing a control plane is an important metric in the assessment of natural attenuation at contaminated sites. For risk-assessment purposes, the mass discharge must be estimated together with a level of uncertainty. We present a conditional Monte Carlo approach that allows estimating the statistical distribution of mass discharge. The approach is based on conditioning multiple realizations of the hydraulic conductivity field on all data available. We jointly determine a first-order decay coefficient in each realization, leading to conditional statistical distributions of all estimated parameters and the total mass discharge. The resulting statistical distribution of contaminant mass discharges can be used in the assessment of risks at the contaminated site. The method is applied to data of hypothetical test cases, which gives the opportunity to compare estimation results to the true field. As concentration data, we account for pointlike measurements obtained in multi-level sampling wells. The obtained empirical distribution of mass discharge crossing the multi-level sampling fence could be well fitted by a log-normal distribution.

1. Introduction

Proving the reduction of contaminant mass discharge in the direction of flow is the main target of assessing natural attenuation. Even though other lines of evidence exist, estimating the total mass discharge itself remains indispensable. Towards this end, two classical methods exist.

The first method is based on concentration measurements obtained in multi-level sampling wells (Borden et al., 1997; King et al., 1999; Kao and Wang, 2001; Kübert and Finkel, 2006). In the given references, the mass discharge crossing the sampling plane is assessed by assuming piecewise constant fluxes. This approach can be interpreted as coarse-interpolation approach, in which the accuracy depends directly on the number of measurement points. In practical applications the spatial density of measurements is often insufficient to obtain reliable results. Many measurements would be needed to ensure that the plume is totally covered.

The second method makes use of integral pumping tests (Schwarz et al., 1998; Holder et al., 1998; Bockelmann et al., 2001, 2003). In this approach, the concentration is measured in a series of pumped wells. The undisturbed concentration distribution is subsequently reconstructed based on assumptions about the concentration distribution (e.g., uniformity in certain spatial directions). The method leads to systematic bias in mixing-controlled reactive transport, since the pumping induces mixing.

As alternative, a new method was proposed by directly measuring the flux of a contaminant in so called passive flux meters (Hatfield et al., 2002, 2004). However, field applications show a great uncertainty of these types of measurement (Stroo et al., 2003), and it may take some time until this approach is suitable for reliable mass discharge estimation.

As important as the estimation of the mass discharge itself is the quantification of the associated uncertainty of the estimation, which so far has seldom be considered. The above mentioned mass discharge estimation techniques do not provide any uncertainty estimate. The uncertainty of these methods may be approximated by additional Monte Carlo simulations. Kübert and Finkel (2006) computed the estimation

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error of various methods in hypothetical test cases but they did not provide a technique of estimating the mass discharge uncertainty from the measurements themselves.

Bakr et al. (2003) proposed inferring the log-transmissivity field from hydraulic head and transient concentration measurements using geostatistical inversion, and propagated the approximate conditional uncertainty of the estimate to performance variables of groundwater management schemes by linearized uncertainty propagation (see also Cirpka et al., 2004). The proposed method could be remodeled to estimate the mass discharge at the site. However, limitations of linearized uncertainty propagation would apply.

To the best of our knowledge Li et al. (2007a,b) have presented the only study estimating the statistical distribution of the mass discharge by a conditional Monte Carlo approach. Each conditional realization of concentration and hydraulic conductivity is based on indicator kriging (Almeida and Journel, 1994) and *p*-field simulation (Froidevaux, 1993).

Our approach shows some similarities with the one by Li et al. (2007a,b). We also obtain the complete empirical distribution of mass discharge crossing a control plane by a conditional Monte Carlo approach. The difference lies in the generation of the conditional realizations by geostatistical inverse methods. In particular, we use the quasi-linear geostatistical approach (Kitanidis, 1995) which was adopted to handle steady-state concentration measurements by Schwede and Cirpka (2009). In contrast to Li et al. (2007a,b), we do not cosimulate conductivity and concentration values. We condition the log-hydraulic conductivity field on all available hydraulic measurements and concentration values available. By this, we guarantee that all estimates of hydrological measures are in agreement with the governing equations of flow and transport, because all calculations in each realization are based on an individual conditioned hydraulic conductivity field.

Our scheme makes use of the same type of measurements as the classical multi-level sampling methods. Fig. 1 gives a schematic view on a multi-level sampling well, which might be used to obtain the data needed. The major difference between our approach and the classical methods lies in the interpolation of the pointlike data. While the classical coarse-interpolation methods only interpolate the measurements of concentration within the control plane, we invert all available data to obtain

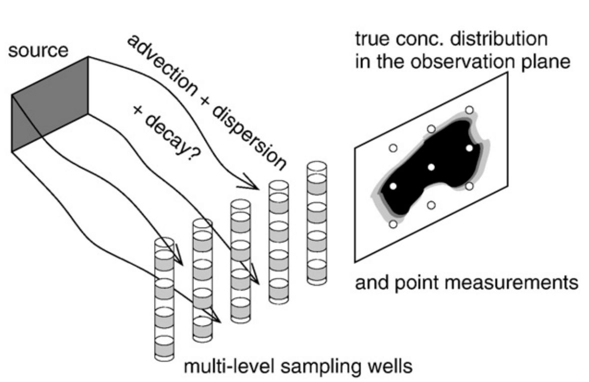

Fig. 1. General set up of the problem. A contaminant is continuously emitted by a source. Further downstream, the solute discharge is measured in a fence of multi-level sampling wells. The true concentration distribution within the observation plane is unknown. Only pointlike measurements exist. What is the total mass discharge and how large is its estimation variance?

estimates of the underlying conductivity field and subsequently compute values of velocity and steady-state concentration within the control plane (Schwede and Cirpka, submitted for publication). This enables us to include other data such as measurements of hydraulic heads, direct estimates of hydraulic conductivity from grain-size analysis, flowmeter tests, pumping tests, and borehole-dilution test data. All of these sources of information may be assimilated to infer the underlying log-hydraulic conductivity field in a geostatistical context. For the conditioning of the unconditional log-conductivity fields on the various types of measurements, we use the quasi-linear geostatistical approach of Kitanidis (1995) with modifications (see Schwede and Cirpka, 2009), but other methods of conditioning conductivity fields on dependent measurements may be used as well (e.g., Hendricks Franssen et al., 2003; Llopis-Albert and Capilla, 2009). Performing a forward simulation leads to conditional distributions of the concentration and specific-discharge fields throughout the domain from which we get a continuous estimate of the mass discharge in the control plane. This procedure is repeated for each realization of the log-conductivity field. The associated uncertainty of the estimation is obtained from the ensemble of conditional realizations.

This paper is organized at follows: Section 2 reviews the governing equations and describes the principle algorithms of the suggested approach. In Section 3 we present the application to hypothetical two-dimensional and three-dimensional test cases. In Section 4 we draw conclusions from our study.

2. Theory

2.1. Governing equations

The total mass discharge J crossing a control area A is given by

$$J = \int_A \mathbf{n}_A \cdot \mathbf{q} c \, d\mathbf{x}, \tag{1}$$

in which $\mathbf{n}_A$ is the unit vector normal to area A, $\mathbf{q}$ is the specific-discharge vector, c is the concentration, and $\mathbf{x}$ is the vector of spatial coordinates.

The specific-discharge vector $\mathbf{q}$ vector in a porous medium is given by Darcy's law:

$$\mathbf{q} = -K \nabla h \tag{2}$$

with the hydraulic conductivity K, and the hydraulic head h.

We consider steady-state groundwater flow without internal sources or sinks, so that the hydraulic head h meets the following partial differential equation (*pde*):

$$-\nabla \cdot (K \nabla h) = 0 \text{ on } \Omega, \tag{3}$$

in which Ω is the domain. We set Dirichlet boundary conditions at the in- and outflow boundaries of the domain, Γ_{in} and Γ_{out}, and no-flow Neumann conditions along the other boundaries, Γ_{no}:

$$\begin{array}{rcll} h & = & h_{in} & \text{on} \quad \Gamma_{in} \\ h & = & h_{out} & \text{on} \quad \Gamma_{out}, \\ \boldsymbol{n} \cdot (K \nabla h) & = & 0 & \text{on} \quad \Gamma_{no} \end{array} \tag{4}$$

for given functions h_{in} and h_{out} along the respective boundaries and normal vector $\boldsymbol{n}$ of the domain. $\Gamma = \Gamma_{in} \cup \Gamma_{out} \cup \Gamma_{no}$ is the