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Screening-level estimates of mass discharge uncertainty from point measurement methods

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ABSTRACT

The uncertainty of mass discharge measurements associated with point-scale measurement techniques was investigated by deriving analytical solutions for the mass discharge coefficient of variation for two simplified, conceptual models. In the first case, a depth-averaged domain was assumed, consisting of one-dimensional groundwater flow perpendicular to a one-dimensional control plane of uniformly spaced sampling points. The contaminant flux along the control plane was assumed to be normally distributed. The second case consisted of one-dimensional groundwater flow perpendicular to a two-dimensional control plane of uniformly spaced sampling points. The contaminant flux in this case was assumed to be distributed according to a bivariate normal distribution. The center point for the flux distributions in both cases was allowed to vary in the domain of the control plane as a uniform random variable. Simplified equations for the uncertainty were investigated to facilitate screening-level evaluations of uncertainty as a function of sampling network design. Results were used to express uncertainty as a function of the length of the control plane and number of wells, or alternatively as a function of the sample spacing. Uncertainty was also expressed as a function of a new dimensionless parameter, Ω, defined as the ratio of the maximum local flux to the product of mass discharge and sample density. Expressing uncertainty as a function of Ω provided a convenient means to demonstrate the relationship between uncertainty, the magnitude of a local hot spot, magnitude of mass discharge, distribution of the contaminant across the control plane, and the sampling density.

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1. Introduction

Contaminant mass flux J [$ML^{-2}T^{-1}$] and mass discharge $\dot{m}$ [MT^{-1}] combine two important features of contaminant risk: concentration C [ML^{-3}] and mobility (e.g., Suthersan et al., 2010). These measurements have been used for a number of site management purposes, including assessments of degradation rates (e.g., Borden et al., 1997; Kao and Prosser, 2001; Kao and Wang, 2000, 2001; King et al., 1999; Semprini et al., 1995; Suarez and Rifai, 2002), characterization of source zones and associated plumes (e.g., Basu et al., 2006, 2009; Einarson and Mackay, 2001; Fraser et al., 2008; Guilbeault et al., 2005; King et al., 1999; Newell et al., 2011), characterization of back diffusion from aquitards (Chapman and Parker, 2005), and assessments of benefits from partial mass removal from DNAPL source zones (Brooks et al., 2008; Cai et al., 2012; DiFilippo and Brusseau, 2008).

Specific methods used to measure J and $\dot{m}$ have been summarized in several publications (e.g., Chen et al., 2014; ITRC, 2010; Kavanaugh et al., 2011; Kübert and Finkel, 2006), and can be divided into two broad categories: point-measurement methods and pumping-measurement methods. Point-measurement methods are based on sampling techniques with relatively small sampling volumes, and most often

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consist either of applications based on multi-level samplers (e.g., Freitas et al., 2011; Guilbeault et al., 2005; Kao and Wang, 2001) or passive flux meters (PFMs) (e.g., Annable et al., 2005; Hatfield et al., 2004). With respect to the former, variations between approaches stem from methods used to estimate the Darcy flux q [LT^{-1}], and equally important, the spatial scale over which those measurements are made. A common criticism of point-measurement methods is the uncertainty that results when they are used to estimate $\dot{m}$ due to the un-sampled regions between measurement locations. In contrast, pumping-measurement methods integrate information over a much larger sampling volume, and thereby minimize the potential for uncertainty due to un-sampled regions between point-measurement locations. Pumping-measurement methods can be sub-divided into two groups: steady-state (Bayer-Raich et al., 2004; Brusseau et al., 2007; Einarson and Mackay, 2001; Holder et al., 1998) and transient methods. In the latter category, the original and most common pumping-measurement method is the integral pump test (Bayer-Raich et al., 2004, 2006; Bockelmann et al., 2001; Schwartz et al., 1998), but other pumping-based approaches have been investigated and used (Brooks et al., 2008; Goltz et al., 2009; Kavanaugh et al., 2011).

The gain in certainty by minimizing un-sampled space in the application of a pumping-measurement method comes at the expense in loss of information about the spatial J distribution. Thus, a trade-off is made between spatial information and the level of uncertainty associated with the measurement of $\dot{m}$. The uncertainty associated with un-sampled space when using a point measurement can of course be minimized by collecting more point measurements to reduce the distance between sampling locations. Increasing the number of samples, however, increases cost.

A number of studies have been completed on point-measurement method uncertainty (Béland-Pelletier et al., 2011; Cai et al., 2011, 2012; Chen et al., 2014; Klammler et al., 2012; Kübert and Finkel, 2006; Li and Abriola, 2009; Li et al., 2007; MacKay et al., 2012; Schwede and Cirpka, 2010; Troldborg et al., 2010, 2012). Two of these studies were based on field trials (Béland-Pelletier et al., 2011; MacKay et al., 2012), two of the studies used flow and transport simulations within Monte Carlo frameworks (Chen et al., 2014; Kübert and Finkel, 2006); two more studies likewise used flow and transport simulations within Monte Carlo frameworks, but simulations were conditioned to field data (Schwede and Cirpka, 2010; Troldborg et al., 2010); and the remaining studies employed various conditional, geostatistical techniques, wherein one or more parameters across the control plane were treated as spatial random variables.

Kubert and Finkel (2006) conducted an extensive Monte Carlo analysis on a hypothetical site to evaluate uncertainty as a function of measurement method, sampling density (S_D), and hydraulic conductivity (K) heterogeneity. As an example of the results obtained, the mean relative error was less than 10% for all levels of heterogeneity using an approach that directly measured flux with $S_D = 5$ pts/m^2. When S_D was reduced to 0.1 pts/m^2, the mean relative error increased, and ranged from ~30% to ~60% for $0.25 \le \sigma^2_{\ln K} \le 4.5$. Their research also noted the uncertainty that may result when combining measurements based on different support volumes, as for example when local scale measurements of K are combined with site-wide average measurements of the hydraulic gradient I. Under this approach, the mean relative error ranged from approximately 40% to 500% for $0.25 \le \sigma^2_{\ln K} \le 4.5$, even using the highest sampling density of 5 pts/m^2.

Kübert and Finkel (2006) used a temporally and spatially constant source of uniform C to generate the contaminant plume in their simulations. The area of the source was ~20% of the model domain cross section, and therefore was more than 20% of the control plane area. As a comparison, Guilbeault et al. (2005) noted that 80% of the plume mass-discharge occurred within 10% or less of the control plane area at three field sites they investigated. The impact of smaller contaminant mass distributions on uncertainty was investigated by Li et al. (2007), as part of a method they demonstrate to quantify uncertainty using empirical mass discharge cumulative distribution functions (CDFs) based on joint geostatistical simulations of random C and K fields conditioned to field measurements. They noted that in the case of $\dot{m} = 319$ g/d, a S_D of 0.1 pt/m^2 yielded a mean relative error of ~20%, but the same S_D yielded a mean relative error of ~180% in the case of $\dot{m} = 15$ g/d. To achieve a ~20% mean relative error for $\dot{m} = 15$ g/d, their results indicated a S_D of ~3 pt/m^2 would be needed. This work was extended by Li and Abriola (2009) who presented a staged sampling strategy, where optimal sample locations were identified by evaluating initial sampling results from mean C, local random variable entropy, and C conditional variance criterion. Compared to sampling densities based on a single sampling event with a regularly spaced grid, a sampling density of half or less was needed based on their staged approach.

Other studies that likewise presented methods to estimate $\dot{m}$ uncertainty using geostatistical simulations of random spatial variables conditioned to field measurements include Cai et al. (2011), Cai et al. (2012), Klammler et al. (2012), and Troldborg et al. (2012). In each case, uncertainty was quantified by generating empirical CDFs of $\dot{m}$. Cai et al. (2011) assumed uniform flow, such that uncertainty stemmed only from the spatial C distribution. This approach was extended in Cai et al. (2012) to include K as a second, independent spatial random variable. In both cases, uncertainty was summarized using boxplot representations of the CDFs. Data from the boxplots was used to calculate a normalized 95% confidence interval (defined as the difference between the 97.5% and 2.5% quantiles, divided by the 50% quantile), which ranged from 35% to 76% for the case studies investigated. Troldborg et al. (2012) calculated mass discharge uncertainty through Bayesian conditional simulations, where C and q were treated as independent random spatial variables, but q was generated from a joint conditional simulation of K and I. The method was applied to a field site with $\sigma^2_{\ln K} = 1.4$, and using sampling networks with $S_D = \{0.32, 0.05\}$ pts/m^2, they estimated $\dot{m} = \{12, 21\}$ g/d total chlorinated ethenes, respectively. The coefficient of variation CV associated with these two estimates were {43%, 74%}, respectively. Klammler et al. (2012) present a stochastic simulation method conditioned to PFM measurements to estimate the CDF of $\dot{m}$ across the control plane. The method was used to estimate uncertainties associated with two PFM deployments: in the first case, $CV = 16\%$ for a site with $\dot{m} = 777$ g/d trichloroethylene using a sampling network with $S_D = 0.4$ pts/m^2; and in the second case, $CV = 7\%$ for a site with $\dot{m} = 19$ g/d uranium using a