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Controlling scaling metrics for improved characterization of well-head protection regions

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SUMMARY

We addressed the value of hydrogeological information on the assessment of the risk that an operating pumping well is polluted. The work considered a heterogeneous aquifer and focused on the statistical characterization of the contaminant mass fraction from a diffused source recovered at the well and the solute arrival times. We explored the role of the key length scales that characterize and control the well capture region and its probabilistic delineation with respect to the contaminant source location and size. The impact of augmenting the data-base of hydraulic information on the reduction of uncertainty associated with the environmental scenario analyzed was then investigated. It was found that obtaining a robust characterization of the target Environmental Performance Metrics (EPMs) depends on the length scale considered. For the sampling scheme considered, the importance of conditioning on the probability distributions of solute mass fraction and travel times is strongly affected by the location of the contaminant source within the probabilistic well catchment. With reference to the characterization of the travel time distribution associated with the recovery of a given mass fraction, the worth of augmenting the hydraulic parameter data-sets tends to decrease with decreasing solute residence time within the well catchment.

1. Introduction

A key aspect in the delineation of wellhead protection regions in the context of groundwater management practice is to provide decisions with quantifiable uncertainty. Uncertainty related to wellhead protection regions is typically due to the lack of exhaustive characterization of the subsurface environment and main process dynamics. Only limited descriptive details are usually available for site characterization and interpretive models adopted to represent system dynamics are based on simplifying assumptions and plagued by incomplete knowledge of governing mechanisms.

Environmental Performance Metrics (EPMs) (e.g., de Barros et al., 2012, and references therein) which are used to ground strategic decisions affecting protection and/or restoration of groundwater resources, are also subject to uncertainty. In the context of source protection, an EPM employed to guide effectiveness of aquifer remediation scheme or well protection protocols could represent human health risk, concentration levels at an environmentally sensitive well/source location, or solute arrival times at a pumping well.

Representing the spatial variability of hydraulic properties such as hydraulic conductivity or transmissivity within a stochastic framework is an appropriate and convenient way to cope with uncertainty stemming from incomplete system knowledge. Stochastic analysis of wellhead protection in randomly heterogeneous aquifers based on the assessment of key elements of distributions of residence times or trajectories of nonreactive solutes directly ties with the concept of intrinsic well vulnerability, as expressed by Frind et al. (2006) and Enzenhoefer et al. (2012, and references therein).

The analysis of the probabilistic delineation of well catchment boundaries and time-related capture zones is typically tackled within a numerical Monte Carlo framework. Other approaches based, e.g., on moment-equations are also found (Lu and Zhang, 2003b; Riva et al., 2006a). Starting from the works of Bair et al. (1991), Franzetti and Guadagnini (1996), and Cole and Silliman (1997), a series of studies are concerned with unconditional (i.e., in the absence of measurements of hydraulic conductivity or

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transmissivity) analysis and aim at providing qualitative and quantitative descriptions of well recharge areas as a function of the degree of heterogeneity of the underlying hydraulic conductivity/transmissivity field. The concept of probability distribution of solute time-of-travel to the well conditional to a given probability of capture is explored numerically by Van Leeuwen et al. (1998) and Guadagnini and Franzetti (1999) through a suite of Monte Carlo simulations and without considering the effect of hydraulic parameter measurements. Riva et al. (1999) explore the nature of the probability distribution of solutes residence times within a purely convergent flow field. This work is then extended by Riva et al. (2009) to include the effect of heterogeneous sorption distribution.

The effect of conditioning on various networks of measurements of hydraulic conductivity/transmissivity or hydraulic head on the quantification and reduction of uncertainty associated with the spatial distribution of probabilistic well catchment and/or time-related capture zones is explored numerically, amongst others, by Vassolo et al. (1998), Feyen et al. (2001), van Leeuwen et al. (2000), Feyen et al. (2002), Bakr and Butler (2005), and Bakr et al. (2006). The impact on uncertainty reduction associated with incorporating different types of lithological and geophysical information within Monte Carlo iterations is illustrated, e.g., by Riva et al. (2006b) and Dassargues et al. (2006).

Numerical solutions of groundwater flow moment equations is also adopted to provide the mean and bounds of uncertainty of well catchment regions for unconditional and conditional systems (Lu and Zhang, 2003b; Riva et al., 2006a). No systematic studies are currently available with reference to (conditional or unconditional) moments of time-related capture zones.

An extensive review of stochastic methodologies that are employed for the delineation of well protection regions in the presence of multiple sources of uncertainties, including recharge and boundary conditions, is presented by Stauffer et al. (2005).

All of the above referenced studies are concerned with the analysis of the effect of conditioning on the spatial pattern of (ensemble) moments or probability distribution of limiting trajectories or residence times within a prescribed probabilistic catchment and consider point injections of solute particles in the system. To the best of our knowledge, only a limited set of these studies present detailed results on the dependence of probability distributions of critical environmental quantities (e.g., travel times conditional to a given solute mass fraction captured by the well) on key length scales associated with source location and the spatial heterogeneity of the system hydraulic parameters and/or conditioning on hydraulic information.

The recent work by Enzenhoefer et al. (2012) builds on these experiences and places the well vulnerability criteria proposed by Frind et al. (2006) in a probabilistic context. Enzenhoefer et al. (2012) perform a numerical Monte Carlo analysis and present probabilistic intrinsic well vulnerability maps following a point contaminant release and associated with (a) the time of arrival at the well of the peak concentration, (b) a measure of the associated peak concentration, (c) the time required to cross a given concentration threshold at the well, and (d) the time of exposure, corresponding to the interval during which the prescribed threshold concentration is exceeded. The authors illustrate their results by way of a synthetic example, where unconditional simulations are juxtaposed to conditional simulations based on a limited set of information on hydraulic head and transmissivity extracted from a reference scenario.

In the general context of environmental protection and risk assessment, Maxwell et al. (1999) and de Barros et al. (2009, and references therein) show how improved site characterization through assimilation of hydraulic conductivity data affects human health risk measures. Uncertainty reduction in solute concentration and travel times has also been investigated in this framework (Rubin, 1991; Rubin and Dagan, 1992; Nowak et al., 2010; de Barros et al., 2012). A key point emphasized in some of the above mentioned works is the importance of the role of key length scales in reducing uncertainty and guiding data acquisition efforts. Maxwell et al. (1999) and de Barros et al. (2009) show how plume-scale and scale of the pumping well capture zone could assist directing characterization efforts within a human health risk context. The significance of the location of the environmentally sensitive target with respect to the contaminant release location is addressed by de Barros et al. (2012) for different EPMs. All these works point out how rational site characterization needs to take into account the relevant EPMs to be modeled and the length scales that define and control the different processes taking place in the aquifer system. Further research is still needed to provide improved and effective understanding of the significance of such length scales in reducing the EPM uncertainty and guiding dynamic data acquisition.

In line with these works, here we focus on (i) the probabilistic characterization of selected EPMs related to drinking well protection practices, and (ii) the way uncertainty associated with these metrics is influenced by relevant length scales of the problems and can be governed through data acquisition. We investigate the value of hydraulic information in the reduction of uncertainty of target EPMs associated with diffuse contaminant sources as a function of the length scales associated with the initial plume and the scale of the catchment induced by the action of pumping. The EPMs we consider are the following: (i) the mass fraction recovered at the well and (ii) the time of first-arrival to the well for given mass fraction. Key research questions we address as a function of the above mentioned length scales include (a) the assessment of the probability distribution of the selected EPMs and (b) the evaluation of the benefit of additional hydraulic data assimilation to the reduction of uncertainty of the EPMs. This allows elucidating the role of the main (dimensionless) length scales that characterize and control the well capture zone and its delineation on the above mentioned EPMs.

2. Formulation

Here, we are interested in evaluating the dependence of the statistics of the fraction of the injected mass arriving at a pumping well on (a) the solute source dimensions and location within the flow domain with respect to the position of the well and with reference to the mean flow direction, and (b) availability of site characterization measurements. To address the research questions posed in the Introduction, we consider flow through a heterogeneous porous formation with a statistically isotropic hydraulic conductivity $K(\mathbf{x})$ and constant porosity ϕ, where a uniform (in the mean) natural base flow takes place. Here, the m-dimensional spatial coordinate system is denoted by $\mathbf{x}(x_1, \ldots, x_m)$. At the location $\mathbf{x}_w$, a pumping well continuously operates with pumping rate Q.

A solute plume of mass M_o is released from an injection zone of volume $\mathcal{V}_o$ at time t_o. The mass M_o is discretized into a finite number (N_p) of particles, each one associated with a mass δm (such that $M_o = \delta m \times N_p$). The metric of interest here is the mass fraction defined as $M_f \equiv M(\mathbf{x}_w, t)/M_o$, with $M(\mathbf{x}_w, t)$ being the mass arriving at the pumping well. By construction $M_f \in [0, 1]$. The mass fraction can be expressed as a function of the solute discharge from the source Q_s (i.e., mass per unit time)

$$M_f(\mathbf{x}_w, t|\mathcal{V}_o^*, t_o) = \frac{1}{M_o}\int_{t_o}^{t} Q_s(\mathbf{x}_w, \tilde{t}|\mathcal{V}_o^*, t_o)d\tilde{t}. \quad (1)$$

$\mathcal{V}_o^*$ being the fraction of $\mathcal{V}_o$ which falls within the well catchment in a given realization of the ensemble. The solute discharge at the well is given by