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Global sensitivity analysis of groundwater transport

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SUMMARY

In this work we address the model and parametric sensitivity of groundwater transport using the Lagrangian-Stochastic Advection–Reaction (LaSAR) methodology. The 'attenuation index' is used as a relevant and convenient measure of the coupled transport mechanisms. The coefficients of variation (CV) for seven uncertain parameters are assumed to be between 0.25 and 3.5, the highest value being for the lower bound of the mass transfer coefficient k_0. In almost all cases, the uncertainties in the macro-dispersion (CV = 0.35) and in the mass transfer rate k_0 (CV = 3.5) are most significant. The global sensitivity analysis using Sobol and derivative-based indices yield consistent rankings on the significance of different models and/or parameter ranges. The results presented here are generic however the proposed methodology can be easily adapted to specific conditions where uncertainty ranges in models and/or parameters can be estimated from field and/or laboratory measurements.

1. Introduction

The three dominant components of contaminant transport by groundwater considered here are: (i) hydrodynamic drivers (i.e., advection and macro-scale dispersion), (ii) mass transfer (i.e., exchange with the immobile zones/phase), (iii) decay/degradation. These three components (or mechanisms) occur simultaneously, and for a linear system are hierarchical: The hydrodynamic components directly influence mass transfer. Advection, macro-dispersion and mass transfer all strongly influence degradation, whereas degradation of a contaminant has no impact on the hydrodynamics or mass transfer; likewise, mass transfer does not influence the hydrodynamics.

The hydrodynamic components of transport in groundwater are strongly influenced on the one hand by the boundary conditions and on the other hand by the underlying heterogeneity of the hydraulic properties (Dagan, 1984, 1989). Although it is common to describe the statistics of hydraulic conductivity by relatively simple models (e.g., log-normal distribution with low to moderate variance, exponential covariance, (Dagan, 1989)) the hydrogeological structure of aquifers can be complex and variability large such that hydrodynamic mechanisms are non-Fickian and the advection–dispersion equation is not applicable (e.g., Dagan et al., 2003; Fiori et al., 2007). Mass transfer is typically described by a simple equilibrium or first-order mass transfer model (Coats and Smith, 1964; Brusseau et al., 1989; Brusseau and Rao, 1990); mass transfer in fractured rock is commonly described as Fickian diffusion between fractures and the immobile water of the rock matrix (Neretnieks, 1980; Cvetkovic et al., 1999; Cvetkovic, 2010). In reality, the mechanisms of mass transfer may be more complex such that the diffusion-controlled exchange is non-Fickian (Havlin and Ben-Avraham, 1987; Giona, 1992). Thus when quantifying expected attenuation for a given aquifer, we are in a position to first define the models for the dominant transport mechanisms and then to infer their parameters by experimental means. Given these tasks and uncertainties, systematic sensitivity analysis are still of considerable practical interest in order to understand the most dominant dependencies.

In this work we address the model and parametric sensitivity of groundwater transport using the Lagrangian-Stochastic Advection–Reaction (LaSAR) framework (Cvetkovic and Shapiro, 1990; Cvetkovic and Dagan, 1994). Furthermore, the 'attenuation index' introduced and defined in our earlier work (Cvetkovic, 2011b) will be used as a relevant and convenient measure of the coupled transport mechanisms. The sensitivity will be carried out as global sensitivity analysis (Saltelli et al., 2000; Sobol, 2001; Sobol and Kucherenko, 2009; Kucherenko et al., 2009; Lamboni et al., 2013) where the so-called Sobol indices as well as derivative-based indices, will be used to quantify the significance of different parameters.

The paper is organised as follows. First, we summarise the analytical modelling framework. Next we define the attenuation index and the global sensitivity indices. Finally, we present and discuss the results of the computations.

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2. Solute transport by groundwater

Consider solute transport by groundwater from a source area $\mathcal{A}$ (Fig. 1). The rate of contaminant release over the entire area $J_0(t)$ [M/T] is assumed given. A mean flow direction is assumed parallel to the x-axis with a mean velocity U [L/T].

The hydrodynamic transport is characterised by a finite (integral) scale denoted as I_x [L]; this scale may be specified as the integral scale of the hydraulic conductivity, or the integral scale of the Lagrangian velocity (Gotovac et al., 2008). With I_x and U, we define a characteristic time used for normalisation in the following as I_x/U.

There are different approaches available for quantifying contaminant transport by groundwater, from numerical to (semi)analytical. For sensitivity analysis it is highly advantageous to use analytical approaches, which are as general as possible in terms of processes and parameters.

Let J [M/T] denote the expected solute discharge across the control plane at location x parallel to the mean flow. For relatively low concentrations, J can be computed by convolution

$$J(x,t) = \int_0^t J_0(t')h(x,t-t')dt' \tag{1}$$

where h [1/M] is the discharge for unit pulse injection. The function $h(t)$ can be computed in the Laplace Transform (LT) domain based on the solute mass balance that is 'upscaled', or averaged, from a single trajectory (stream tube) to multiple trajectories as (Appendix A):

$$\widehat{h}(x,s) \equiv \langle \widehat{\gamma} \rangle = \int_0^\infty e^{-\tau s(1+\widehat{g})} f(\tau;x)d\tau \equiv \widehat{f}[s(1+\widehat{g});x] \tag{2}$$

where $f(\tau;x)$ [1/T] is the probability density function (PDF) of water travel time τ, g [1/T] is the so-called 'memory function' that characterises mass transfer (exchange) processes, 'hat' denotes LT, and s is the LT variable. Note that h in (1) is in effect a 'transfer function', decomposed by (2) into basic processes of advective transport controlled by heterogeneous structure and hydrodynamics through f, and the mass transfer controlled by small-scale diffusion and/or sorption through g. The transport solution (2) derives from the mass balance equations formulated along three-dimensional trajectories with advective water travel time as an independent variable (the LaSAR approach). Details of relating concentration, flux and discharge along stream-tubes (trajectories) are given in Cvetkovic and Dagan (1994).

Both f and g are aquifer-specific and can take different forms. In this study, we shall use two most general analytical forms of these functions. Specifically, we shall use the tempered one-sided stable (TOSS) density as summarised in Appendix B (Cvetkovic, 2011a); this density can be reduced to most of the known and generic

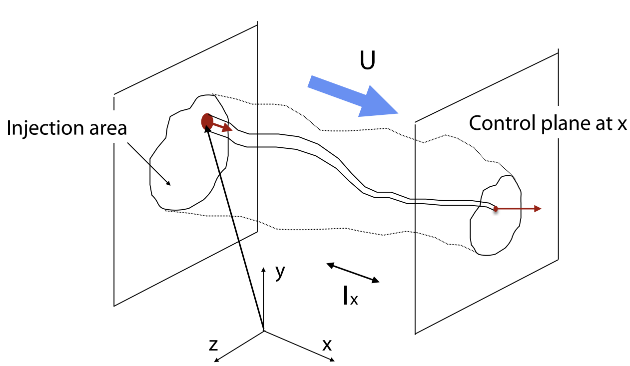

Fig. 1. Problem configuration sketch.

analytical water travel time PDFs used in hydrological transport. For the mass transfer processes, we employ a multi-rate formulation where the rates are distributed as a truncated power-law in form of a Pareto type I distribution (Appendix C).

With f (13) of Appendix B and g (18) of Appendix C, expression for h (2) writes:

$$\widehat{h}(x,s) = \exp\left\{ca^\alpha - c[a + s(1 + A \cdot {}_2F_1(1,\nu;\nu+1;-s/k_0))]^\alpha\right\} \tag{3}$$

which has six parameters: a, c, α, ν, A and k_0. a, c and α are parameters dependent on the hydrodynamics and structure, related to the first two moments of travel time $\overline{\tau}$ and σ_τ^2 in (14); note that in the following we shall use the coefficient of variation $\zeta \equiv \sigma_\tau/\overline{\tau}$ in stead of the variance. The parameters A, k_0 and ν control the mass transfer (exchange) processes.

A wide range of special cases can be obtained from (3) relevant for unconsolidated as well as for consolidated (fractured, dual-porosity) porous media, which makes the LaSAR formulation (2) or (3) particularly appealing. It is instructive to list special (limiting) cases of the expression (3) as follows.

- If $A = 0$ we have hydrodynamic transport only which incorporates mean advection and a macro-dispersive process as quantified by ζ; $\alpha \neq 1/2$ and a finite imply non-Fickian (but not anomalous) transport.
- If $A = 0$ (hydrodynamic transport only), and $a \to 0$, we have anomalous hydrodynamic transport (i.e., all moments of f above zeroth are not defined), in form of the one-sided stable (Levy) distribution (Hughes, 1995).
- If $A = 0$ (hydrodynamic transport only), and $\alpha = 1/2$, then f is an inverse-gaussian PDF and the transport is a solution of the advection–dispersion equation with injection and detection in the flux. Parameters a and c are related to a mean groundwater velocity U and a macro-dispersivity α_L by (15) in Appendix B; note that in this case $\zeta = \sqrt{2\alpha_L/x}$ where x is the longitudinal distance.
- If $A = 0$ (hydrodynamic transport only), and $\alpha \to 1$, we have plug flow with the mean water residence time $\overline{\tau}$, i.e., $h \to \delta(t - \overline{\tau})$ whereby $\zeta \to 0$.
- If $A = 0$ (hydrodynamic transport only), and $\alpha \to 0$, we have the Gamma distribution that has been often used in hydrological transport; parametrisation in this case (and a related case of the exponential PDF also used frequently in hydrological transport) are given in Cvetkovic (2011a).
- If $A \neq 0$, $k_0\overline{\tau} \gg 1$, we have hydrodynamic transport (Fickian or non-Fickian) coupled with linear equilibrium sorption; if $\alpha \to 1/2$, the hydrodynamic transport is governed by the ADE.
- If $A \neq 0$, $\nu > 2 - 3$ we have hydrodynamic transport (Fickian or non-Fickian) coupled with first-order linear (kinetic) mass transfer; if $\alpha \to 1/2$, the hydrodynamic transport is governed by the ADE. The limiting 'memory function' in this case is $g(t) \to Ak_0e^{-tk_0}$.
- If $A \neq 0$, $\nu = 1/2$ we have hydrodynamic transport (Fickian or non-Fickian) coupled with Fickian diffusion and sorption into immobile zones of limited capacity; if $k_0 \to 0$, we have Fickian diffusion and sorption into immobile zones of unlimited capacity.
- If $A \neq 0$, $\alpha = 1/2$, $\nu = 1/2$ and $k_0 \to 0$ we have the classical model of ADE transport in dual-porosity media with Fickian diffusion into an unlimited matrix (Cvetkovic et al., 1999).

Eq. (3) is the simplest and most general (semi)analytical formulation of groundwater transport for arbitrary A, $0 < \alpha < 1$ and $\nu > 0$, particularly suitable for parametric as well as model sensitivity analysis. h (3) depends on six parameters: $\overline{\tau}$, ζ, α, A, ν and k_0. Out of these, α and ν would be more related to model sensitivity