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IDENTIFYING CONTAMINANT RELEASE CONDITIONS TO REDUCE UNCERTAINTY IN PLUME SPREADING AND DILUTION IN HETEROGENEOUS AQUIFERS

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Summary. The initial width of contaminant plumes has a key influence on expected plume development, dispersion and travel time statistics. In past studies, initial plume width has been perceived identical to the geometric width of a contaminant source or injection volume. A recent study[1] on optimal sampling layouts for minimum variance prediction of contaminant concentration showed that the largest uncertainty in predicting plume migration stems from the total hydraulic flux through the source area, overwhelming other sources of uncertainty along the further travel distance in a large range of situations. This result points towards a missing link between source geometry and plume statistics, which we denote as the effective source width. We define the effective source width by the actual, rather than the expected hydraulic flux, through the source area. It is a stochastic quantity that may strongly differ from the actual geometric source width for small sources, and becomes identical only at the limit of wide sources (approaching ergodicity). We derive its stochastic moments in order to explore the dependency on scale and to define the limit of ergodic contaminant source (not plume) width. Effective source width is a contribution to dispersion since it is linked to the prediction variance of plume width. It is separable from the dilution part of dispersion similar to spreading and the uncertainty in predicting the center of mass is separable from dilution. We show that the chance of plumes to be consumed in a single hot-spot of mixing and dilution depends strongly on its overall width. Therefore, its knowledge will improve the prediction of contaminant dilution and mixing. In addition, we illustrate that if the effective source width at a given site is known rather than the geometric width, predictions of plume development, d ispersion and travel time statistics would greatly increase in predictive power. The results of this study also offer advice in what situations sampling efforts should focus primarily on release conditions rather than on other sources of uncertainty.

1 INTRODUCTION

Stochastic description of contaminant transport is a necessity since full characterization of natural porous media, such as aquifers, is an unfeasible task. Many past studies have provided powerful tools to predict contaminant transport, based on the ensemble behavior of spatial and temporal moments[2]. In these studies, the initial width of a plume (e.g., the dimension of the contaminant source) is directly related to fundamental characteristics such as plume ergodicity and is a key parameter in predictions of plume development, dispersion, dilution and mixing. Up to date, the initial plume width has been perceived as identical to the width of a source or of an injection volume[3 4]. A recent study by Nowak *et al.* (2009)[1] has identified optimal sampling strategies for minimum variance prediction of contaminant concentrations at an environmentally sensitive location. In their resulting optimal designs, the largest number of samples is spent in order to investigate certain hydraulic phenomena directly at the source location rather than transport phenomena further down-gradient. The authors proposed that the major source of uncertainty addressed by these optimal sampling schemes is the total volumetric water flux passing through the source area.

The importance of focused volumetric water flux in the spreading of contaminants in saturated porous media has been shown in the literature[5]. These authors showed, through numerical and analytical approaches, how the convergence of streamlines within a zone can enhance the transverse mixing of the plume. When flow is focused within a high permeability zone, streamlines converge and then diverge again. When streamlines are closer together, a higher diffusive transfer of solute mass is faciliated, contributing to lateral plume dilution. The opposite occurs when flow is blocked by a low permeability zone. Experimental evidence was also shown[6 7], where the squeezing of contaminant plumes in high permeability inclusions was investigated. Based on their experimental observations,the authors[7] defined a source equivalent width which is a function of the volumetric injection rate. We will show that the effects of streamline convergence/divergence are much more relevant if it occurs at the contaminant source location because it influences the entire transport regime (mass flux, plume width, etc) further downstream. The above evidence and discussion indicates that there is a missing link between a given source geometry and the resulting width of a plume. The basic idea of the current work is to differentiate between the actual geometric width of the source zone and its effective width, related by what we denote as the source efficiency. We define source efficiency as the ratio of actual versus the expected hydraulic flux passing through the geometric area of the source. The effective source width is an uncertain quantity that results from the stochastic nature of total discharge through a cross-sectional area where the contaminant source is located. Hence, its theoretical statistical moments can be derived from the integral statistics of specific discharge within the source volume. The results by Nowak *et al.* (2009)[1] indicate that effective source width is a key parameter in the prediction of contaminant transport. We hypothesize that, if the effective source width at a given site was known, predictions of contaminant plume development would increase in predictive power.

The aim of the current contribution is to support this hypothesis through the use of closedformed analytical expressions for effective source width derived from the governing equations of flow. We verify its validity with high-resolution numerical Monte-Carlo in a 2D depth-averaged setting.

2 The Concept of Effective Source Width

2.1 Mathematical Formulation

In the following, we will differentiate between the geometric width of the source zone (w_{sz}) and its effective width (w_{eff}). We consider an incompressible, fully saturated, two-dimensional steady-state flow within a confined, depth-averaged aquifer. Let $\mathbf{x} = (x_1, x_2)$ represent the cartesian coordinate system with velocity field $\mathbf{v}$ satisfying Darcy's Law. The mean flow is taken along the direction x_1. Consider a contaminant line source (width equal to w_{sz}) perpendicular to the direction of mean flow with fixed concentration c_o. The effective source width, w_{eff}, is defined with the aid of the continuity equation:

$$w_{eff} = w_{sz}\frac{Q_{sz}}{\langle Q_{sz}\rangle}, \tag{1}$$

where Q_{sz} is the volumetric water flux passing through the source zone:

$$Q_{sz} = \int\limits_{W_{sz}} q_1(x_1, x_2) b dx_2 \,. \tag{2}$$

Here, b denotes aquifer depth, $q_1(x_1, x_2)$ the specific discharge passing through the source zone and $\langle\cdot\rangle$ the ensemble expectation. Taking the geometric source width as a given quantity in equation (1), the randomness lies in the source efficiency denoted as η:

$$\eta = \frac{Q_{sz}}{\langle Q_{sz}\rangle} \,. \tag{3}$$

For an unbounded two-dimensional aquifer with uniform-in-the-average flow, $\langle Q_{sz}\rangle$ is given by:

$$\langle Q_{sz}\rangle = J T_G w_{sz} \,, \tag{4}$$

where J is the mean hydraulic gradient in the x_1 direction and T_G is the geometric mean of transmissivity. Equation 4 applies because T_G is the effective transmissivity for infinite, two-dimensional aquifers[2]. In addition, we can express Q_{sz} in terms of the stream function values that bound the edges of the geometrical source (namely, ψ_s and ψ_i). Now we can re-write equation (3) as follows:

$$\eta = \frac{\psi_s - \psi_i}{J T_G w_{sz}} \,. \tag{5}$$

The stochastic moments of η will follow as well as its verification with Monte-Carlo simulations.

2.2 Illustrative Example

In order to install the importance of source efficiency for predicting contaminant concentrations, we first demonstrate, visually, its general impact on transport problems by performing a Monte-Carlo transport analysis with 20,000 realizations. The physical-mathematical formulation, boundary conditions and numerical implementation details are provided in the literature[1]. For each realization, we computed the total volumetric flux passing through the source zone to obtain the respective source efficiency η and the effective source width w_{eff}. From that ensemble, we extracted two subsets, one with effective source width $w_{eff} > 3/2 w_{sz}$ and another with $w_{eff} < 2/3 w_{sz}$. The respective concentration mean and variance fields, of the total Monte Carlo set and extracted subsets, are shown in Figures 1.a-c and 2.a-c.

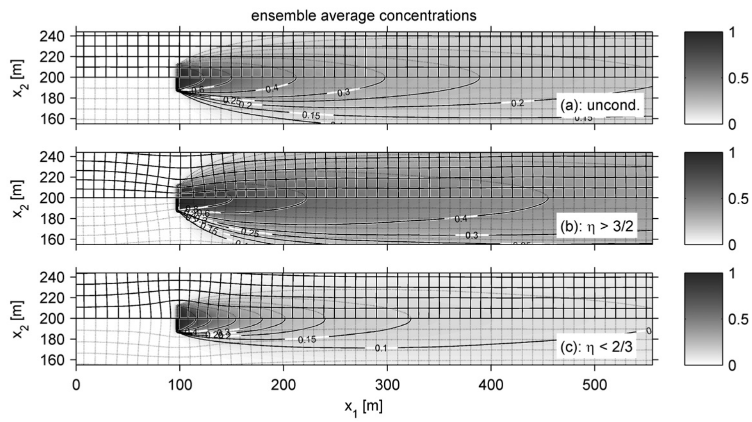

Figure 1: Impact of effective source width, see equations (1) and (3), on ensemble mean concentration (base case scenario). Simulation results for an isotropic exponential covariance model: (a) Concentration mean of all realizations with source efficiency larger than 3/2. (b) Same for source efficiency smaller than 2/3.

3 Stochastic Moments of Source Efficiency

3.1 Analytical Development

From equation (5), the source efficiency η results from the stochastic nature of total discharge Q_{sz} (defined in terms of the bounding stream function values) through a non-ergodic cross-sectional area. In two-dimensional (depth-averaged) aquifers, the statistics of the bounding stream function values offer a mathematically straightforward way to obtain analytical first-order approximations to the first and second stochastic moment of effective source width[9]. The mathematical development is straightforward, since well-known methods used for the stochastic groundwater flow equation can be transferred to the corresponding streamline equation[9]. Since w_{eff} is proportional to η, we now focus on the stochastic moments of η. We start by taking the expected value of η:

$$\langle \eta \rangle = \left\langle \frac{Q_{sz}}{J T_G w_{sz}} \right\rangle = 1. \tag{6}$$

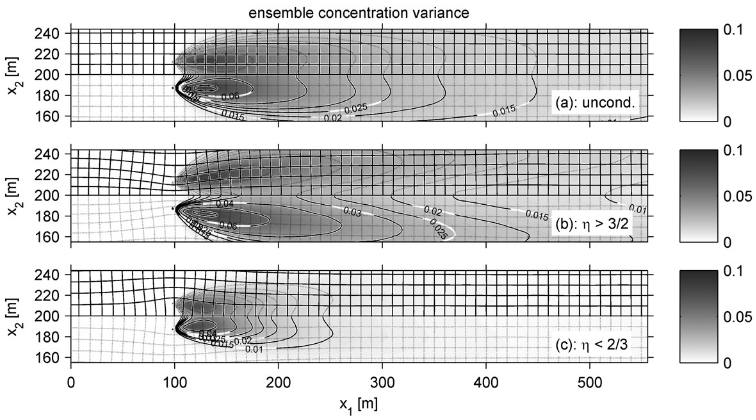

Figure 2: Same as in Figure 1 but for concentration variance.

It follows that, of course, the geometric source width is the best estimate of initial plume width in absence of site-specific data. The variance of η is expressed as:

$$\begin{aligned}\sigma_\eta^2 &= \frac{1}{J^2 T_G^2 W_{sz}^2} Var\left[\psi_s - \psi_i\right] \\ &= \frac{2}{J^2 T_G^2 w_{sz}^2} \Gamma_{\psi_s \psi_i}\,,\end{aligned} \tag{7}$$

where $\Gamma_{\psi_s\psi_i}$ is the stream function variogram value for the bounding values ψ_s and ψ_i. The stream function variogram $\Gamma_{\psi_s\psi_i}$ is evaluated at the longitudinal and transversal lag-distances r_1 and r_2 such that $\Gamma_{\psi_s\psi_i} \equiv \Gamma_{\psi,2}(r_1 = 0, r_2 = w_{sz})$. The subscript "2" in $\Gamma_{\psi,2}$ denotes transversal direction. A formal derivation for the stream function variogram, along with the necessary assumptions, is given in de Barros and Nowak (2010)[9]:

$$\Gamma_{\psi,2}\left(r_1, r_2\right) = T_G^2 \Gamma_{h,1}\left(r_1, r_2\right), \tag{8}$$

where $\Gamma_{h,1}$ correponds to the longitudinal hydraulic head variogram. Equation (8) reflects a rotation of $\Gamma_{h,1}$ by ninety degrees with a scaling factor given by T_G^2. For the given lag distances (dictated by w_{sz}), this leads to:

$$\sigma_\eta^2 = \frac{2}{J^2 w_{sz}^2} \Gamma_{h,1}(w_{sz}, 0)\,. \tag{9}$$

After replacing $\Gamma_{\psi,2}$ by the head variogram $\Gamma_{h,1}$, we can draw on existing analytical solutions. In our case, we will use (for demonstration) the first-order approximation[8], derived for the isotropic exponential covariance model. Figure (3) illustrates how the variance of η decays with increasing values of w_{sz}. Equation (9) quantifies to what degree small sources are more affected by the uncertainty in w_{eff} than wide sources. It indicates the transition to ergodic source width (rather than ergodic plume width), where effective and geometric source width become almost identical (when the variance become negligible, around 100 transverse integral scales as shown in the figure).

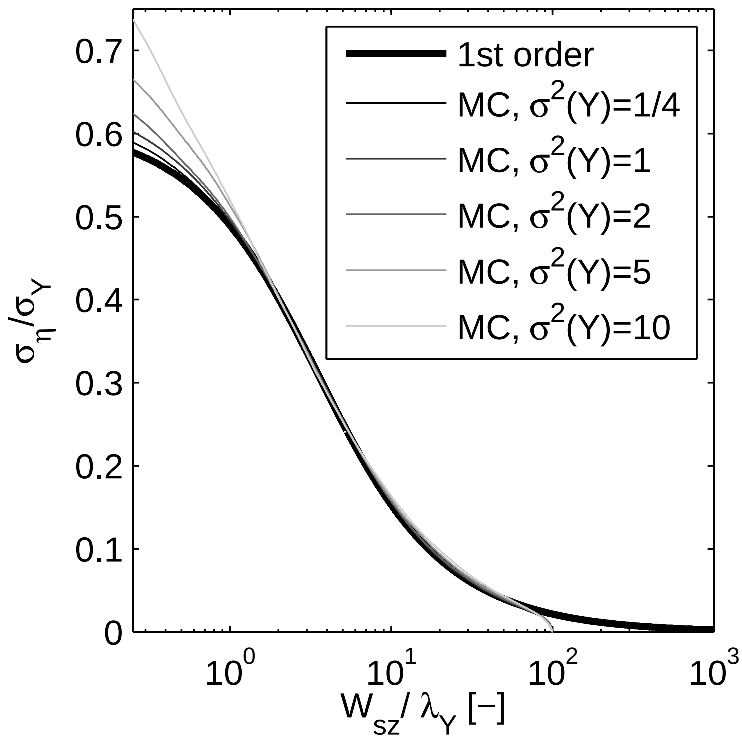

Figure 3: Dependence of source efficiency standard deviation on normalized geometric source width, comparison of analytical first-order expression and results from Monte-Carlo analysis.

3.2 Verification by Monte-Carlo Simulation

Dagan (1985)[8] found that first-order approximations for hydraulic head covariances are quite accurate even for higher variances of log-conductivity σ_Y^2. Since our solution is based on the head variogram, we expect it to be robust even for high values of σ_Y^2. For comparison and verification purposes, we performed an accompanying numerical evaluation by Monte-Carlo analysis of the streamline equation. The results are taken from 20,000 realizations in a domain sized $100\lambda \times 100\lambda$, at a grid spacing of 10 elements per λ. Technical details as well as choice of parameters are provided in an ongoing work by de Barros and Nowak (2010)[9]. Results were obtained for different values of σ_Y^2 in order to detect the range of vailidity in σ_Y^2. The volumetric fluxes were evaluated at hypothetical source zones of various width, placed in the center of the domain to minimize boundary influences.

The agreement between the analytical and numerical curves for the limiting case of $\sigma_Y^2 \to 0$ is perfect ($\sigma_Y^2 = 0.0001$, results not shown here). Overall, the analytical solution is very robust even at values of $\sigma_Y^2 > 1$. The deviations with increasing σ_Y^2 are conform with recent head and velocity statistics published in the literature: A higher variance of η for small geometrical width coincides with the fact that the local variance of specific discharge scales more than linearly with σ_Y^2. The sudden drop to zero close to 100 integral scales is an artifact of the bounded numerical domain used in our Monte-Carlo analysis. The analytical result for the variance of source efficiency reaches an asymptotic value of zero only for $w_{sz} \to \infty$.

4 Summary

An analytical solution for the statistics of η was formally derived up to first-order. The solution was succesfully compared with numerical Monte-Carlo simulations. We showed how the variance of η decreases with the geometrical source width and reaches ergodicity $(w_{sz} \to \infty)$ when w_{sz} is equal to approximately 100 transversal integral scales. The obtained closed-form solution proved robust for values of σ_Y^2 far above unity.

In summary, local hydraulic conditions in the area of the area of contaminant release have strong impact on plume characteristics. The current paper provides a simple approach to increase the predictive power of existing analytical solutions. As an outlook of future work, the analytical solution, as well as the results given here, could be particularly useful to quantify the spreading effects due to inclusions of high (or low) permeability and are currently being investigated[9]. Up to now, the observations[9] are in agreement with the results published[6] where the impact of inclusions on spreading of contaminants was shown experimentally.

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