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On the link between contaminant source release conditions and plume prediction uncertainty

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ABSTRACT

The initial width of contaminant plumes is known to have 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 on optimal sampling layouts (Nowak et al., 2009) showed that a significant portion of uncertainty in predicting plume migration stems from the uncertain total hydraulic flux through the source area. 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 ratio between the actual and expected hydraulic fluxes times the *geometric* source width. The actual hydraulic flux through the source area is given by individual realizations while the expected one represents the mean over the ensemble. It is a stochastic quantity that may strongly differ from the actual geometric source width for geometrically small sources, and becomes identical only at the limit of wide sources (approaching ergodicity). We derive its stochastic ensemble moments in order to explore the dependency on source scale. We show that, if the effective source width is known rather than the geometric width, predictions of plume development can greatly increase in predictive power. This is illustrated on plume statistics such as the distribution of plume length, average width, transverse dispersion, total mass flux and overall concentration variance. The analysis is limited to 2D depth-averaged systems, but implications hold for 3D cases.

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 the plume's spatial and temporal moments (for an extensive review see Rubin, 2003). 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 (e.g., Rubin et al., 1994; Andricevic and Cvetkovic, 1998; Dentz et al., 2000).

Up to date, the initial plume width has been perceived as identical to the width of a source or of an injection volume (e.g., Dentz et al., 2000; Fiorotto and Caroni, 2002; Schwede et al., 2008). A recent study by Nowak et al. (2010) has identified optimal sampling strategies for minimum variance prediction of contaminant concentrations at environmentally sensitive locations located down-gradient of the source. 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

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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 is shown in Werth et al. (2006) and Valocchi and Nakshatrala (2009). These authors showed, through numerical and analytical approaches, how the convergence of streamlines within some given zone can enhance the transverse mixing of the plume. When flow is focused within a high permeability zone, streamlines converge and then diverge again. While the 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 in Rahman et al. (2005) and recently by Rolle et al. (2010), where the squeezing (or channeling) of contaminant plumes in high permeability inclusions was investigated. Based on their experimental observations, Rahman et al. (2005) defined a source equivalent width which is a function of the volumetric injection rate (in a similar fashion to the asymptotic catchment zone width of a pumping well which is defined by the ratio between the background flow and pumping rate). Recently, Valocchi and Nakshatrala (2009) showed the sensitivity of transversal spreading on the contaminant source location. They illustrated how spreading is enhanced if the source is located within high- or low-permeability zones. In this paper, 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.) farther downstream. Strong field evidence for the relevance of local field hydraulic conditions at the source zone can be found in Frind et al. (1999), where the plume leaving a DNAPL source was unexpectedly thin and could almost not be detected.

The above evidence and discussion indicate 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 (in each realization) versus the expected (ensemble mean) hydraulic flux passing through the geometric area of the source. In real situations, the actual hydraulic flux through the source can be obtained by collecting head and hydraulic conductivity measurements around the source area. Consequently, this data could be used to condition simulations, see Ch. 3 of Rubin (2003). The effective source width is an uncertain quantity that results from the stochastic nature of total discharge through the 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. (2010) indicate that effective source width is a key parameter in the prediction of contaminant transport. In their work on concentration probability functions, Schwede et al. (2008) conceptualized the uncertainty of flow rate in the source, but approximated it by point-scale velocity statistics. However, velocity at a single point has different statistics than the integral discharge over the cross-sectional area of a non-point source. Hence, further efforts are necessary to investigate the properties of source hydraulics. We hypothesize that, if the effective source width at a given site was known, predictions of contaminant plume development (i.e., total mass flux, plume length, width, dispersion, dilution and concentration variance) would increase in predictive power. The aim of the current work is to support this hypothesis through the use of closed-formed analytical expressions for effective source width derived from the governing equations of flow. We verify its validity with high-resolution numerical Monte-Carlo flow and transport simulations of characteristic plume statistics depending on the effective source width in a 2D depth-averaged setting.

Section 2 introduces the concept of effective source width along with its mathematical formulation. We also define a parameter denoted source efficiency η, which according to our definition, absorbs all randomness of effective source width. Section 3 derives the statistical moments of source efficiency. The effects, significance and implications of the results with respect to plume prediction and its spatial moments are illustrated in Section 4. Finally, conclusions are given in Section 5.

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 (other release conditions are discussed in Section 4.5). 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:

$$Q_{sz} = \int_{w_{sz}} q_1(x_1, x_2) b dx_2. \tag{2}$$

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 Eq. (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:

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