

A time dependent mixing model to close PDF equations for transport in heterogeneous aquifers



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ABSTRACT

Probability density function (PDF) methods are a promising alternative to predicting the transport of solutes in groundwater under uncertainty. They make it possible to derive the evolution equations of the mean concentration and the concentration variance, used in moment methods. The mixing model, describing the transport of the PDF in concentration space, is essential for both methods. Finding a satisfactory mixing model is still an open question and due to the rather elaborate PDF methods, a difficult undertaking. Both the PDF equation and the concentration variance equation depend on the same mixing model. This connection is used to find and test an improved mixing model for the much easier to handle concentration variance. Subsequently, this mixing model is transferred to the PDF equation and tested. The newly proposed mixing model yields significantly improved results for both variance modelling and PDF modelling.

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1. Introduction

Predicting the transport of groundwater contaminants remains a demanding task, especially with respect to the heterogeneity of the subsurface, the large measurement uncertainties, and the increasing impact of human activities on groundwater systems (WWAP, 2012). Hence, a risk analysis also includes the quantification of the uncertainty in order to evaluate how accurate the predictions are.

It is well known from papers published in the last decades that a major source of uncertainty associated with predicting contaminant concentrations is the lack of detailed information about the spatial heterogeneity of the hydraulic conductivity in the subsurface (see e.g. Burr et al., 1994; Gelhar and Axness, 1983). A long standing approach to deal with this uncertainty is the stochastic parameterisation of the hydraulic conductivity through random space functions with statistics inferred from field and laboratory data. Via flow and transport equations, the contaminant concentrations being modelled are random functions too. Their statistics may be inferred from Monte Carlo ensembles of transport simulations, done for realisations of the random hydraulic conductivity, by stochastic perturbation approaches, or by the probability den-

sity function (PDF) method, which received an increased attention during the last decade (Suciu et al., 2016).

The moment approach uses transport equations of the concentration moments consistent with the geostatistical representation of the aquifer's heterogeneity. If this heterogeneity is statistically homogeneous, the equation for the first moment, which is the mean concentration, has the following characteristics: The highly heterogeneous and spatially fluctuating groundwater velocity is replaced by an ensemble averaged velocity field and the effect of the fluctuating velocity on the transport is modelled by an enhanced dispersion called macrodispersion or ensemble dispersion (Gelhar and Axness, 1983). But in general, the mean behaviour differs from that of a specific plume in a single aquifer. See Fig. 1 for a comparison between the mean concentration and a concentration obtained from a simulation in a specific velocity field realisation. Only if the hydraulic conductivity has finite correlation lengths and the plume has sampled a representative part of the aquifer, it becomes ergodic and its transport behaviour can be modelled by the ensemble averaged behaviour, described above. In a first step, possible deviations from the mean behaviour can be quantified by the concentration variance. It is transported by the same processes as the mean concentration, thus it is advected by the averaged velocity field and dispersed by an enhanced macrodispersion. But concentration variance is also generated by mean concentration gradients and simultaneously it is destroyed by dissipative processes, which

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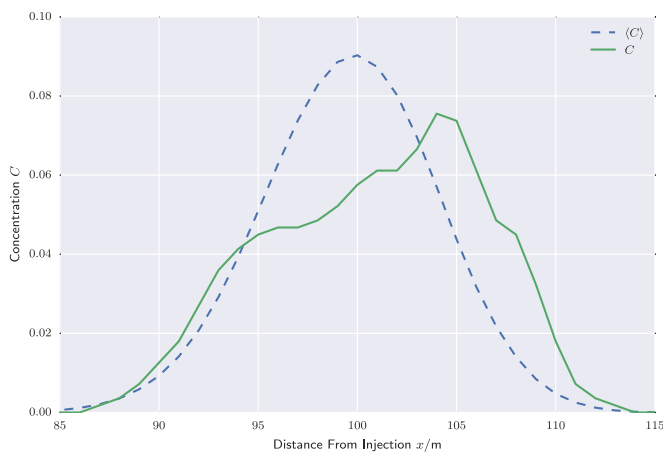


Fig. 1. A measure is needed to quantify how good the mean concentration $\langle C \rangle$ approximates the actual concentration C , since the difference can be significant.

are created by small-scale fluctuations in the velocity field. In order to calculate the influence of these small-scale fluctuations on the concentration variance, a so-called closure model is needed.

In the field of turbulence modelling, where very similar transport equations are used, different approaches exist for such closure models (e.g. Tennekes and Lumley, 1972). Up to this point, the adoption of these approaches to groundwater transport modelling has been hampered by the vastly different flow conditions prevalent in both fields. Contrary to most other problems where turbulent flows are more challenging, the roles are reversed here. The strong mixing induced by turbulent flows causes this closure problem to be easier to tackle. The mixing induced by heterogeneities in the groundwater flow is slower and changes significantly in time and is therefore more difficult to model. Dentz et al. (2000) have shown, the mechanism which generates the physical mixing in a given aquifer realisation is more reliably described by the effective dispersion coefficients in comparison to the ensemble dispersion coefficients, which correspond to the turbulent diffusion coefficients. The effective dispersion is small at early times and increases only slowly with time. Therefore, concentration gradients at early times are steep and may remain steep for prolonged times, which in turn prevents the smoothing of concentration fluctuations and preserves concentration uncertainty. Andričević (1998) proposed a mixing mechanism based on a time variable effective length scale which, in principle, could be determined experimentally. Kapoor and Gelhar (1994a, 1994b) derived a transport equation for the concentration variance, including local dispersivity and macrodispersive transport. By neglecting the local dispersivity, the results from Dagan (1982) could be derived. But it was concluded that even very small local dispersivities create a qualitatively different behaviour compared to the zero local dispersivity case, as the local dispersivity is the only mechanism which can reduce the variance. They used an approach developed for turbulent flows to model the variance dissipation, created by the local dispersivity. Furthermore, analytical solutions for the long-time behaviour of the concentration variance were derived. These results were confirmed for globally integrated variances by numerical simulations (Kapoor and Kitanidis, 1997).

If the predictions made by a contaminant transport model are to be used for risk analysis, even more information than the mean concentration and the variance is needed. Risk thresholds, regulated e.g. by an environmental agency (WWAP, 2012), can only be factored in by the so-called exceedance probability (e.g. Andričević and Cvetković, 1996). It depends on the complete one-point probability density function (PDF) of the concentration. The concentration variance, as discussed above, can only be used to calculate

a first estimation of the exceedance probability (de Barros et al., 2011). Even if such estimation would be an acceptable approximation, rare events or extreme values cannot be mapped by the mean concentration and the concentration variance alone. This limitation stems from the fact that by using only the first two statistical moments, namely the mean and the variance, a Gaussian shape for the concentration PDF is implied. Such a distribution is short-tailed and therefore excludes the possibility of rare events. Yee and Chan (1997) analysed a large set of experimental data from tracer tests in the turbulent atmosphere. From this analysis they identified a collapse of higher-order concentration moments, which means that the higher-order moments can be expressed through lower-order moments. Srzic et al. (2013a) applied such an analysis to the transport of solutes in groundwater and also found a collapse. This might be a promising way of computing the concentration PDF from the mean concentration and the concentration variance.

The first studies applying such a PDF framework to the transport in groundwater used a β distribution, fully characterised by two parameters, to fit the concentration PDF in a non-Gaussian way (Fiori, 2001; Fiorotto and Caroni, 2002). Cirpka et al. (2008) extended the assumption of a β -shaped PDF to some special cases of reactive transport by mapping the statistics of conservative transport to those of mixing-controlled reactions. Srzic et al. (2013b) concluded that β -shaped PDFs only match the true PDF for low heterogeneities. By strictly assuming a multivariate Gaussian random velocity field and by assuming that the PDF of the centre of mass of the solute is also Gaussian, (Dentz and Tartakovsky, 2010) derived a formula for the concentration PDF without need to solve a PDF evolution equation. Their approach consists of mapping the PDF of the random centre of mass of the plume, assumed to be Gaussian, onto the concentration PDF. A similar approach, using a stream function coordinate system, was further developed by Cirpka et al. (2011). A “Lagrangian concentration” framework for calculating the integrated PDF, the cumulative distribution function (CDF), was presented by de Barros and Fiori (2014). They derived a semi-analytical equation for the concentration CDF by assuming a small plume size and a normally distributed and statistically stationary conductivity field with low to mild heterogeneity. Compared to the β -CDF, both models perform similar. A review on assumed β -PDFs and mapping random variable approaches is given by Fiori et al. (2015).

A more flexible approach – the PDF method – is investigated in this study. This approach yields an equation for the whole PDF of the concentration and thus makes no assumptions about the shape of it. Another major advantage of the PDF approach is the possibility to include mass transfer, like chemical reactions or radioactive decay, even in case of nonlinear reactions. This intriguing property of the PDF approach is possible by assuming that the mass transfer solely depends on the concentration (Fox, 2003; Pope, 1985; Succi et al., 2015b). The crux of these PDF methods is finding a mixing model which describes the transport of the PDF in the concentration space. We refer to Celis and Figueira da Silva (2015) for a recent review of mixing models.

The term “mixing” will be used from now on with a precise meaning, as in turbulence literature (Celis and Figueira da Silva, 2015), which, although related, is different from its meaning in stochastic sub-surface hydrology, where it is associated with the effective dispersion coefficient (Dentz et al., 2000). The latter is the diffusion coefficient of the stochastic process modelling the transport, centred on the actual plume centre of mass. It differs from the diffusion coefficient of the process centred on the centre of mass averaged over the ensemble of velocity realisations, i.e. the ensemble dispersion coefficient describing the spreading of the solute plume (Dentz et al., 2000), by the diffusion coefficient of the

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