



Water Resources Research

RESEARCH ARTICLE

10.1002/2015WR017525

Kev Point:

 Debate on stochastic subsurface hydrology

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Citation:

Fiori, A., V. Cvetkovic, G. Dagan, S. Attinger, A. Bellin, P. Dietrich, A. Zech, and G. Teutsch (2016), Debates—Stochastic subsurface hydrology from theory to practice: The relevance of stochastic subsurface hydrology to practical problems of contaminant transport and remediation. What is characterization and stochastic theory good for?, *Water Resour. Res.*, 52, 9228–9234, doi:10.1002/2015WR017525.

Received 9 MAY 2015 Accepted 9 NOV 2016 Accepted article online 18 NOV 2016 Published online 21 DEC 2016

Debates—Stochastic subsurface hydrology from theory to practice: The relevance of stochastic subsurface hydrology to practical problems of contaminant transport and remediation. What is characterization and stochastic theory good for?

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Abstract The emergence of stochastic subsurface hydrology stemmed from the realization that the random spatial variability of aquifer properties has a profound impact on solute transport. The last four decades witnessed a tremendous expansion of the discipline, many fundamental processes and principal mechanisms being identified. However, the research findings have not impacted significantly the application in practice, for several reasons which are discussed. The paper discusses the current status of stochastic subsurface hydrology, the relevance of the scientific results for applications and it also provides a perspective to a few possible future directions. In particular, we discuss how the transfer of knowledge can be facilitated by identifying clear goals for characterization and modeling application, relying on recent recent advances in research in these areas.

1. How Far Have We Come?

The emergence of stochastic subsurface hydrology stemmed from the realization that spatial variability of aquifer properties (primarily permeability K) has a profound impact on solute transport. Heterogeneity is characterized by much larger scale than the pore scale and the seemingly erratic variation of K and the uncertainty of its distribution called for its modeling as a random space function, which renders the fluid Darcian velocity and the concentration random as well.

The first decade of development of stochastic modeling dealt primarily with statistical properties of $Y=\ln K$ (accepted at that time as being univariate normal of mean $\langle Y \rangle = \ln K_G$ and variance σ_Y^2 [e.g., Freeze, 1975]) on one hand and the solution of the flow and transport for weak heterogeneity ($\sigma_Y^2 < 1$) on the other (see, e.g., the monographs by Dagan [1989], Gelhar [1993], and Rubin [2003]), building on the macrodispersivity concept in Fickian regime. The following three decades, the ones of concern to the present debate, witnessed a tremendous expansion of the literature, covering a variety of topics. To mention a few: modeling of structures by various models, e.g., facies indicator variograms and transition probability; fractures and soil unsaturated properties characterization; heads and velocity spatial distribution, their upscaling and use for solving stochastically the inverse problem; transport of reactive solutes, adaptation of random walk techniques, numerical simulations of plumes in highly heterogeneous formations, and nonergodic effects. Each of these topics deserves a separate debate and in view of the present limited scope, we focus our contribution to the one which we regard as central on one hand and ripe for application on the other: transport of solutes in natural gradient flow.

We further focus the scope to the realistic case of 3-D heterogeneity and the ensuing flow and transport. In contrast, we regard two-dimensional models as exploratory theoretical tools motivated by numerical convenience; when they are viewed as a result of upscaling to regional scale, they require anyway solving first for 3-D. Furthermore, our approach is "bottom up," as initially envisaged by the proponents of stochastic models: the starting point is the heterogeneity statistical characterization (achieved by field investigation), the next step is the derivation of the random velocity field by solving the equations of flow and, finally, solving the

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local ADE transport equation which encapsulates the combined effects of advection and local dispersion (which can be generalized to incorporate reactions as well). This approach is physically motivated on one hand and applicable to long-term prediction on the other: spreading of contaminants is a slow process, which may take tens to thousands of years, whereas characterization of structure can be carried out in a relatively short time and at reasonable cost. Furthermore, field survey along the projected plume movement may reveal spatial variations which have to be incorporated in model prediction. This approach is in contrast with "proxy" models, e.g., multirate transfer, which postulate a mechanism characterized by a few parameters which cannot be related directly to the structure and have to be identified with the aid of transport experiments.

Our basic approach to model transport is the Lagrangian one (known as particle tracking in its numerical version), by which solute particles are followed along the trajectories of the fluid (advection) supplemented by a "Brownian" motion component representing local (pore-scale) dispersion. Thus, quantifying of transport reduces to the derivation of the trajectories pdf, after solving the flow problem to derive the random velocity field. For natural gradient flows and steady state (approximations valid for slowly varying flow in space and time), \mathbf{V} is approximated as uniform in the mean, i.e., $\langle \mathbf{V} \rangle = \mathbf{U} = const$.

The simplest and earliest solutions were obtained for weakly heterogeneous aquifers $(\sigma_Y^2 < 1)$, in conjunction with the field tests at the Borden and Cape Cod Sites [Mackay et al., 1986; LeBlanc et al., 1991]. Using a perturbation expansion in the log conductivity fluctuation, it was found that at first-order in σ_Y^2 the mean concentration $\langle C(\mathbf{x},t)\rangle$ satisfies an upscaled ADE with constant advective coefficient U and time dependent longitudinal macrodispersivity coefficient α_L . The latter grows with time and stabilizes at the value $\sigma_Y^2 I$ after a "setting time" and then the ADE becomes a Fickian equation. In particular, the longitudinal plume mass distribution m(x,t) satisfies the 1-D ADE with coefficients U and α_L . It is emphasized that even within this simple approach, prediction requires identification of the key structural parameters σ_Y^2 and I, which are aquifer specific.

These simple results can be readily applied to modeling of aquifer transport for weakly heterogeneous aquifers, after characterization of the Y statistics. Thus, they may serve in order to determine the solute mass arrival and the concentration of an effluent at a control plane (the outlet), or a well which captures the entire plume (with neglect or approximate accounting of the radial flow effect). Simple results were also obtained for other relevant quantities, like, e.g., the statistical moments of local or space-averaged concentrations.

Many aquifers are moderately or strongly heterogeneous ($\sigma_Y^2 > 1$), as is the case for the MADE site ($\sigma_Y^2 \cong 6.6$) [Boggs et al., 1992]. The transport behavior is different: plumes are no more Gaussian and characterization by macrodispersivities and the use of the associated ADE is not appropriate. It is convenient to characterize transport by the BTC (breakthrough curve) at fixed control planes at x, in terms of the solute particles travel time τ from the injection zone to x. While in the Fickian regime the τ pdf is inverse Gaussian, its application for $\sigma_Y^2 > 1$ is not warranted. The MADE site field data have stimulated a large body of research, which was summarized by Zheng et al. [2011]. While the topic of flow and transport in highly heterogeneous aquifers is still under active research, a recently developed model, denoted as MIM (multi-indicator model), consisting of an ensemble of blocks of different Y, associated with a SCA (self-consistent approximation) to solve flow and transport, was found to lead to good agreement with the MADE field measurements [Fiori et al., 2013; Cvetkovic et al., 2014]. The model explains effects which are not present for weak heterogeneity: the long BTC tail caused by large residence time in blocks of low conductivity and the early arrival time due to channeling effects [Fiori et al., 2006]. The model relies entirely on the identified permeability structure, with no fitting of parameters. We surmise that this model, or even its further simplified version, is in a stage close to application toward determining the mass arrival at outlets which capture the entire plume.

2. How Relevant Are the Advances of the Last 30 Years to Practical Problems?

Stochastic subsurface hydrology has led to a change of paradigm, representing a "revolution" (in the terminology introduced by *Kuhn* [1962]) in the field. Many fundamental processes have been clarified, and the principal mechanisms have been identified, introducing a new paradigm: heterogeneity has a crucial impact on groundwater flow and transport and has to be accounted for. However, the research findings of the last 30 years have not impacted significantly the common practice, and routine applications are nowadays often carried out along the old, deterministic paradigm. An attempt to adapt it for transport in heterogeneous formations consists in using a constant longitudinal macrodispersivity value drawn from an "universal" graph representing α_L as function of the distance covered by the solute plume, based on compilation of field data.

We have demonstrated recently that data do not support this approach, which leads to erroneous prediction [Zech et al., 2015b].

There are a few reasons for the lag between research and applications, such as the increased economic effort required by the stochastic analyses as compared with the "standard" techniques, the resistance of the legislation and regulators to deal with probabilistic analyses, the lack of professionals with adequate training on stochastic techniques, to mention some (a few problems have been discussed in a debate forum published by *Stochastic Environmental Research and Risk Assessment*, vol. 18, 4, 2004).

Among the principal problems facing applications is that aquifers are of heterogeneous structure, requiring data that are costly to acquire, such as statistics of *K* and its spatial correlation. However, the issue of reducing time and costs was tackled in the last 20 years by the development of innovative technologies. One group of them are the direct push (DP) technologies [Dietrich and Leven, 2006] which now enable a time and cost efficient site characterization of shallow unconsolidated aquifers, which are typical for contaminated sites in flood plains. In particular, hydraulic DP tools as the DP slug test [Butler et al., 2002] and DP injection logger [Dietrich et al., 2008; Liu et al., 2009] allows nowadays a fast assessment of the spatial variability of permeability. The suitability of these tools was demonstrated at different test sites [Lessoff et al., 2010; Bohling et al., 2012]. Further promising approaches for the determination of the required parameters of the permeability distribution are the interpretation of continuous pumping test data [e.g., Dagan and Lessoff, 2011; Zech et al., 2015a] or the oscillatory pumping test [e.g., Rabinovich et al., 2015]. In addition, efforts have been taken to determine optimal design of experiments [e.g., Geiges et al., 2015]. This opens the opportunity to acquire the needed data also in deeper and consolidated aquifers. But the new innovative technologies are not yet well established and their further development and incorporation in practice is a challenging task.

Thus, practical tools guided by the stochastic paradigm are few, although the last years have seen a promising increase of them, for instance in the form of stochastic moduli attached to popular codes (e.g., Monte Carlo parametric uncertainty and/or random generation of conductivity in conjunction with MODFLOW). The main problem is still how to properly use those tools and how to feed the codes with the right parameters, which brings back to the above characterization issue. Even the use of "classic" parameters like the longitudinal dispersivity α_L are often not based on the advances in stochastic subsurface hydrology; the latter has delineated the limitations of the upscaled ADE (see previous section) and the role of α_L , and it has provided limits of applicability depending on the particular goal at hand. However, these limitations are seldom considered in practice, leading to incorrect and misleading modeling exercises. Besides the aforementioned lack of training, an additional cause is related to the research community which sometimes has concentrated on very specialized topics, quite remote from applications.

Last but not least, we should also mention obstacles posed by yet unsolved research problems, which are still under active research, e.g., transport under radial flow in heterogeneous media, as well as dilution, non-linear reactions, biodegradation, oxidation, to mention some.

3. What Are the Important Future Directions?

The previous sections emphasize several problems that we face when applying stochastic subsurface concepts to practical problems, from the open scientific questions to issues related to characterization and the associated costs. Although most researchers in the field would agree that we still need to better understand processes governing transport and transformation (especially in strongly heterogeneous aquifers), with a parallel advancement of characterization techniques, our emphasis here is on how to effectively relate characterization and predictive modeling.

Given the complexity of subsurface transport processes and data limitations, and considering the current status of the art of the knowledge and tools, a broader use of stochastic models for groundwater transport requires their appropriate "adjustment" to primary application objectives, along a "goal-oriented" approach. The latter consists in focusing the characterization (e.g., resolution, spatial coverage, parameters to be considered) and the modeling (e.g., conceptualization, complexity, scale) on the relevant aspects leading the particular application (or goal) at hand, with typical goals being: What is the risk of exceeding a given concentration at a target point (well), or within a given area? Is natural attenuation relevant in reducing this

risk? How long should one pump from a well, or a battery of wells, in order to reduce this risk below a certain threshold?

We briefly illustrate the above points by considering the problem of risk assessment from existing or potential groundwater contaminations, which is probably one of the most frequent problems encountered at present in practical consulting. The regulatory framework commonly builds on the *source-path-receptor* concept where the adequate representation of subsurface heterogeneity is essential in many respects [*Environmental Protection Agency (EPA)*, 2006]. The aspects related to the source and the receptor are of paramount importance for applications; for instance, the architecture of the source zone, which constitutes the external forcing for any predicting model, has a large impact on the level of contamination and the transport processes along the flow path. However, in the following we focus for the sake of brevity on the *path* component of the above chain, which pertains to the fate of contaminant, from the source to the receptor, which is also subject to high uncertainty.

A specific challenge in the analysis of the flow path is the prediction of extremes like the very fast and the very slow transport paths within a heterogeneous flow field. The "fast" paths are essential in applications like *risk assessment* in proximity of water exploitation or ecologically sensitive sites, where early contaminant arrival times (e.g., the 5% quantile of the breakthrough curve) are of prime interest [e.g., *Andricevic and Cvetkovic*, 1996; *de Barros and Rubin*, 2008]. Advanced numerical methods can eventually solve this kind of problems using adequately large sets of realizations, but the inference of the geostatistical models underlying them is still a weak point. The early arrivals are mainly determined by the connectivity of the porous medium [see, e.g., *Fiori and Jankovic*, 2012], and an efficient characterization should focus on it, starting, e.g., from the simple assessment of the integral scale of the highly permeable zones. The same is true for the modeling tool, which should be tailored for capturing the fast components of flow [see, e.g., *Whittaker and Teutsch*, 1999]. Unfortunately, the available hydraulic characterization methods are not specifically sensitive to detect such connected paths, and appropriate statistical models which address those features are still under development.

In turn, the "slow" flow components are relevant to applications dealing with *remediation*, and in such case knowledge of contaminant mass transfer into low-permeability zones (either by advection or diffusion) is of prime importance [e.g., *Haggerty and Gorelick*, 1994; *Dekker and Abriola*, 2000; *Berglund and Cvetkovic*, 1995]. The spatial density and connectivity of the low conductivity elements, and the mass exchange between them and the faster flows, needs to be properly characterized for remediation-related applications, like, e.g., pump and treat.

Another frequently asked question in practice is: How far downstream of the source is a certain contaminant going to move? This leads to the widely applied concept of *self-purification [Environmental Protection Agency (EPA)*, 1998] of groundwater, where contaminants are removed due to a coupled effect of advection, retention, and transformation (e.g., microbial degradation) [*Cvetkovic*, 2011]. Regulatory acceptance of natural attenuation is commonly based on the proof of a contaminant plume to be steady state in time and on the space mass distribution and/or the solute mass-flux decreasing along the mean flow direction [*Bayer-Raich et al.*, 2006]. Even though of highly economical relevance, we do not have at present the knowledge on how to predict the natural attenuation potential, for example the maximum plume length for a given solute contamination in a given environment. For instance, focusing on microbial degradation, self-purification is governed by local mixing processes, e.g., between the electron donor and receptor, which are in turn triggered by macrodispersion [e.g., *Zarlenga and Fiori*, 2014]. Hence, we need to understand how dilution and the self-purification capacity are related to heterogeneity to assess general vulnerability of existing groundwater resources. Existing stochastic transport models need to be adapted to this purpose and applied for assessing potential attenuation of most important contaminant classes, based on uncertain (site-specific or generic) information [*de Barros et al.*, 2015].

In most applications of groundwater transport, it is desirable to use more than one tool that preferably overlap and at the same time are complementary. Ideally, analytical and numerical tools need to be combined. These tools shall capture the dominant transport mechanisms of (randomly varying) advection, retention (mass transfer), and transformation (degradation, decay). The analytical stochastic models have matured, can account for the dominant mechanisms, and are suitable for estimating prediction uncertainty. Numerical tools are currently well advanced although subsurface heterogeneity still poses a significant challenge

to their use in routine applications. Parallel implementation and combination of numerical and analytical tools that is goal-oriented (i.e., adapted to the specific application goals as noted above) is likely to be the most promising avenue for future applications.

Subsurface hydrology is a highly fragmented area of research where many different approaches have been presented in the literature over past decades, many with little reference to data and real systems. Moreover, subsurface hydrology is a research area without clearly defined common issues and also suffering from knowledge gaps. Above all, the cooperation among researchers working at different world sites has the potential to ensure a focus on resolving most important issues. Taking greater advantage of the progress in this application area may significantly help to spread and adapt more routine implementation of state-of-the-art stochastic approaches in subsurface hydrology.

4. Postscript

We are grateful for the opportunity to summarize our views on the relevance of stochastic subsurface hydrology for engineering applications. After reading the contributions by *Cirpka and Valocchi* [2016], *Sanchez-Vila and Fernandez-Garcia* [2016], and *Fogg and Zhang* [2016], we find a general consensus on the need to introduce concepts and tools of stochastic subsurface hydrology into applications, most noteworthy for uncertainty analysis (e.g., Monte Carlo), including the conceptual model (i.e., epistemic uncertainty) which is often a critical element in groundwater models. In particular, we share a common view with *Cirpka and Valocchi* [2016] on the need for reliable, "off-the shelf" implementation of stochastic methods in industrial-standard codes, including clear, "good practice" guidelines. Such codes and guidelines would help practitioners to assess modeling uncertainty due to incomplete knowledge of hydraulic properties as well as initial and boundary conditions.

The stochastic framework allows for more flexibility in modeling subsurface transport, but requires an adequate characterization of subsurface properties. New methodologies for characterization are currently available, including powerful geophysical methods, however better protocols are required to guide practitioners and researchers in performing field investigations. Such protocols would result in more robust data acquisition and interpretation, making characterization less subjective and dependent on the operator. This point has been emphasized, although from slightly different perspectives, by all the three contributions to the debate. We are indeed convinced that more stringent protocols and guidelines, together with continuously improved education in stochastic hydrogeology, are necessary conditions for making the stochastic approach more accessible in practice and a key development to improve modeling performance in applications.

Unsurprisingly, some of our views diverge from the views of other debaters, notably on the role of analytical solutions. According to *Cirpka and Valocchi* [2016] analytical solutions "do not offer much help in real-world applications"; we believe that analytical solutions can indeed be helpful in a variety of ways, from benchmarking numerical codes to scoping calculations and screening analysis, in addition to their pedagogical and intrinsic value when conditions for their use in real-world applications are met. Furthermore, our view on the MADE experiment and the relevance of non-Fickian transport models in highly heterogeneous aquifers differs from the view expressed by *Sanchez-Vila and Fernandez-Garcia* [2016].

We agree with the general conclusion of *Fogg and Zhang* [2016] that a sound geologic characterization of the subsurface, including aquitard structures is important in developing adequate site models. We do not share the pessimism of *Fogg and Zhang* [2016] however on the applicability of stochastic subsurface hydrology. We believe that *Fogg and Zhang* [2016] greatly underestimate the role of heterogeneity length scale and overestimate the role of the hydraulic conductivity variance. In particular, *Fogg and Zhang* [2016] argue that the interpreted increase in dispersivities with transport distance [e.g., *Neuman*, 1990] can be explained by a hypothesized increasing hydraulic conductivity variance σ_Y^2 with an increasing transport scale. Such a hypothesis however is inconsistent with the recent findings of *Zech et al.* [2015b] who present a detailed analysis of field data from more than 70 field experiments and show that the increase in dispersivities with scale is not supported by available tracer test data. We believe that the applicability of stochastic methods in subsurface hydrology will depend primarily on how well these methods are adapted to the specific modeling goal for any given site, rather than on the level of variability in the hydraulic properties.

In spite of these and perhaps some other differences, we all appear to share a common vision, one of "greater engagement by the scientific community to bridge the gap between research and applications." As emphasized in our debate, further progress in bridging this gap requires more systematic "goal-oriented" approaches with "adaptive complexity" in characterization and modeling that on the one hand are always supported by data (evidence) and on the other are adapted to clearly defined application objectives.

Acknowledgments

This paper does not analyze any new data.

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