

Parameterizing macro-dispersivity: first pick a length scale

Brian Berkowitz (ed.)

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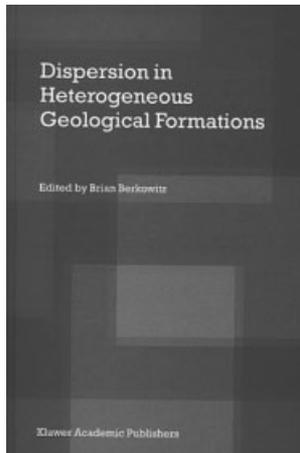
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Dispersion in Heterogeneous Geologic Formations, Brian Berkowitz, edited by Brian Berkowitz.

Despite much previous success in hydro-geologic fieldwork and modelling, the system does remain mostly hidden from human observation. As such, many scientists are still actively engaged in applying new tools and models to understanding solute transport through geologic formations. A focus of current research is the scaling behaviour of many common hydraulic parameters, including porosity, conductivity and Fickian transport parameters (e.g. diffusion and dispersion).

Scale sensitivity in these hydraulic system parameters is revealed when choosing a fixed measurement resolution but increasing the measurement support volume. In such scenarios, one usually finds parameter values that depend on the measurement window. If a plot of parameter values against the measurement scale shows one or more plateaus, the medium has one or more length scales. Every plateau corresponds to a particular volume, known as the representative elementary volume (REV).

A 'Homogenization Theory' provides traction in explaining why parameters follow an asymptotic approach to these plateaus. According to this theory, the observed heterogeneous medium is simplified by replacement with an 'effective' homogeneous medium. Rather than making physical measurements within this domain, effective, or macro-system, parameters are determined through field or laboratory experiments. This is the basic idea behind the definition of effective porosity values, effective conductivity values or macro-dispersion values. In practice, however, the Homogenization Theory does not result in effective parameter values that accurately reproduce the system behaviour.

Macro-dispersion parameters are of particular interest, with selected values often overestimating the real mixing processes in heterogeneous formations. The difference between measured and effective values is explained by physical constraints on the length scale at the experimental site, which is frequently too short to reach the REV's effective parameter at the actual asymptotic limit. Instead, pre-asymptotic, or non-ergodic, values are measured, which represents one realization of the transport behaviour in these complex and heterogeneous formations.

Pre-asymptotic transport behaviour in geologic media is the focus of several papers assembled by Brian Berkowitz in the new book *Dispersion in Heterogeneous Geologic Formations*, reprinted from the 2001 special issue of Jacob Bear's (ed.) journal *Transport in Porous Media* **42**, (1–2). This volume contains 11 articles, each offering a scholarly and unique perspective on a subterranean system that many of us will never observe.

The contributions to this book are organized into theoretical versus field- or laboratory-based work, yet the first article is further distinguished

from the rest by providing treatment of stochastic flow behaviour. The remaining ten articles focus on the realizations of heterogeneous transport. Though the reader does not need to understand the intricate mathematical details of transport equations, an elementary primer may help provide appreciation for mathematical techniques employed by the authors. An important reminder is the understanding that transport equations are often solved numerically rather than analytically. Further, a method technique useful for small perturbations is to compute a power series expansion about the unperturbed solution. This is referred to as the perturbation expansion technique.

The first article, by *Bonilla and Cushman*, steps quickly into the mathematics used to tackle heterogeneous systems, and the authors use a perturbation expansion technique to analyse the stochastic flow problem. More interestingly, they contend that flow patterns in heterogeneous media are essentially determined by the log-conductivity value *gradients* rather than the log-conductivity values themselves, particularly as a small perturbation parameter. The perturbation parameter is defined by the observation scale, which may vary from small to large, divided by the correlation length. In principle, the perturbation expansion theory works only on small parameters. Hence, the expansion terms for this perturbation parameter may only account for pre-asymptotic effects given that, at the asymptotic regime, which is a longer length scale, the value might no longer meet the criterion of 'small'. Limitations to small perturbations can be overcome by using renormalization group analysis, as presented by *Sposito*. Again, though knowledge of numerical methods will help the reader with these first articles, they were written so that the concepts are conveyed separate from the equations.

The features of pre-asymptotic transport behaviour are the focus of the remaining nine articles. *Pannone and Kitanidis*, for example, reveal that for very long particle transport times, when travelling through heterogeneous formations, particle displacements are correlated with a limited number of other transport steps. In steady-state conditions the central limit theorem applies and macro-dispersion coefficients for the mean concentration can be identified. For transient conditions, however, the central limit theorem does not hold. A quantity displaying that fact is the concentration covariance. It is a global measure for

plume non-uniformity representing deviations around the mean concentration. *Pannone and Kitanidis* determined concentration covariances for the Cape Cod Tracer Experiment (1985–88) and used them for interpolation of data in a kriging approach in order to account for the pre-asymptotic plume non-uniformity. Their work implies that results of stochastic theories should be used very carefully. Though they provide us with *a priori* information over an ensemble of all possible realizations in a probabilistic framework, only under ergodic conditions do the mean values describe a single realization.

In order to gain reasonable concentration results that capture to some extent the pre-asymptotic behaviour, appropriate mean values have to be defined and the variances have to be considered, as demonstrated by *Fiori*. He used the concentration covariance to measure the centre of fluctuations quantitatively from streamline to streamline. The corrected macro-dispersion coefficients are equivalent to so-called effective dispersion coefficients that describe a more realistic mixing of the plume for finite times. *McLaughlin and Ruan*, who examined the applicability of classical macro-dispersion concepts to situations where small- and large-scale velocity variations are both present, also study non-ergodic transport. They observed scale interactions between the two scales that could not be modelled by standard macro-dispersion theory.

Supporting work by *Silliman and Zheng*, as well as by *Labolle and Fogg*, found pre-asymptotic plume behaviour in experiments. *Silliman and Zheng* performed a two-dimensional laboratory experiment, where the effective conductivity of the heterogeneous medium was in good agreement with theoretical predictions of stochastic theories. The measured spatial moments, however, showed deviations from the theoretical values of asymptotic theories.

At larger spatial scales, *Labolle and Fogg* simulated solute migration in an alluvial aquifer. Large-scale variability was modelled by a series of spatially distributed hydro-facies representing the dominant structures. Within each facies, effective parameters accounted for sub-scale variability. Their results demonstrated that the solute mainly moves within a more conductive channel network; however, an increase of molecular diffusion increased the net flux of solute into less permeable facies. This meant that mass was held back and clean-up times could

essentially be determined by the constrained flux rates. This effect cannot be modeled by macro-dispersion fluxes.

Koplik demonstrated that transit-time solute distributions were useful as non-invasive surface tools to characterize subsurface multipole reservoirs. Even if stochastic theories show limitations in the predictive power of one single realization, this non-invasive technique was very useful for the single value context. As *Guadagnini and Neuman* pointed out, the support of measurements is uncertain, and/or the data are corrupted, by experimental, often invasive, and interpretive errors. The errors and uncertainties render the flow and transport stochastic. In other words, stochastic theories are capable of describing how uncertainties or the lack of knowledge are propagating through the system.

So far, heterogeneous media with one or more length scales and pre-asymptotic behaviour with respect to these scales has been studied. However, there are also natural formations that show evolving scales with respect to the measurement resolution. For these media, no finite length scale exists and classical dispersion theories based on the central limit theorem have to fail. In other words, the system is pre-asymptotic over all scales. In the framework of a more general limit theory, stable laws so-called Levy-distributions were derived by

Levy. They are governed by fractional transport equations that reduce only in special cases to standard advection–dispersion equations. *Benson et al.* state that the traditional advection–dispersion equation fails to predict concentration profiles of a conservative tracer in the Columbus Air Force Base aquifer (MADE) because the aquifer shows non-stationary conductivity values. Using fractional transport equations the profiles could be reproduced with remarkable accuracy over different time and length scales. Similarly, *Berkowitz and Scher* found anomalous transport behaviour for solute transport through systems with evolving scales.

Even if these articles do not present a complete theory of transport in heterogeneous porous media, they give insight to the actual status of the complex topic of non-ergodic transport behaviour. And with actual status, the status of 1999 is meant. According to the editor, Brian Berkowitz, the authors were requested to display the mathematics to a minimum. However, some of articles are very technical and basic introductions are often missing. Therefore, the book is not well suited for readers who are not familiar with transport theories in heterogeneous media. It offers the expert comprehensive information over the broad spectrum of situations where one is confronted with non-ergodic transport behaviour and where the concept of macro-dispersion fails.