

LA-UR- 08-4833

Approved for public release;
distribution is unlimited.

Title: The scale dependence of dispersivity in multi-faces heterogeneous sediments
(This is the English translation of the Chinese paper)

Author(s): Shu-ning DONG¹, Zhenxue Dai², Jing-sheng LI³
1. School of Environmental sciences and Engineering,
Changan university, Xian 710054, Shaanxi, China
2. EES-6 Earth and Environmental Sciences Division
Los Alamos National Laboratory
3. Xian Research Institute, CCRI. Xian 710054, Shaanxi,
China

Intended for: J. of Hydrogeology and Engineering Geology (in Chinese)



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

The scale dependence of dispersivity in multi-faces heterogeneous sediments

Shu-ning DONG^{1, 2}, Zhenxue DAI³, and Jing-sheng LI²

(1. School of Environmental sciences and Engineering, Chang'an university, Xian 710054, Shannxi, China; 2. Xian Research Institute, CCRI . Xian 710054, Shaanxi, China; 3. Los Alamos National Laboratory, NM 87545, USA)

Abstract: Based on a general global covariance function of log conductivity in multi-faces sediments we developed the macrodispersion coefficient equations for the solute transport in three-dimensional domain. Then we derived the longitudinal dispersivity to show the scale dependence of this parameter. With an example, the time evolution trends and the relative contributions of the auto- and cross-facies transition terms to the macrodispersion have been discussed. Sensitivity analysis indicates that the values of the longitudinal dispersion coefficient are positively correlated to facies mean length and the difference of the mean log conductivity between different facies. The longitudinal dispersivity coefficient also shows clearly a linear dependence on the global variance of the log conductivity in the multi-facies sediments.

Key words: dispersivity; multi-face heterogeneous sediments; scale dependence; macrodispersion coefficient equations

1. Introduction

The Lagrangian approach was introduced in stochastic modeling of solutes transport in porous media by Dagan (1989) and has received significant attention since, as reviewed by Rubin (1995, 2003). Early work with the Lagrangian approach assumed that log conductivity could be represented by a single, finite integral scale representing the spatial correlation of log conductivity. Recently, attention has been focused on representing log conductivity across different scales so that the integral scale may be neither finite nor single valued (Zhang, 2002). Some work has sought to characterize the scaling of the variance and correlation of log conductivity, or alternatively the macrodispersivity, through considering a compendium of field observations and scaling experiments, and has posed general scaling model. Some work has used these and other models for the scaling of spatial correlation of log conductivity and illustrated the resulting behavior of solute spreading (e.g. Dagan, 1994; Cushman et al., 1994; Di Federico and Neuman, 1998). In most of the prior work there has not been a strong link between the model for the spatial correlation of log conductivity and the geology it is supposed to represent.

The Lagrangian approach requires a model for the univariate and spatial bivariate moments for log conductivity. Recent work presented such models for bimodal domains (Rubin, 1995), multimodal domains (Lu and Zhang, 2002), and hierarchical multimodal domains (Ritzi et al., 2004). Here we use the multimodal models for developing the log conductivity covariance function.

In this paper the Lagrangian approach will be used to derive the macrodispersion coefficients for conservative solute transport through multi-modal heterogeneous

formations. The attractiveness of the approach here is that it offers the possibility of relating the macrodispersion coefficients to the sedimentary architecture. We first consider the geology, specifically that of unconsolidated multi-modal sediment resulting from fluvial deposition (see Figure 1). We discuss how the spatial statistics for log-conductivity at different scales are related to the multi-modal sediment across a range of scales. We then study how the mean lengths of sediment facies affect macrodispersivity.

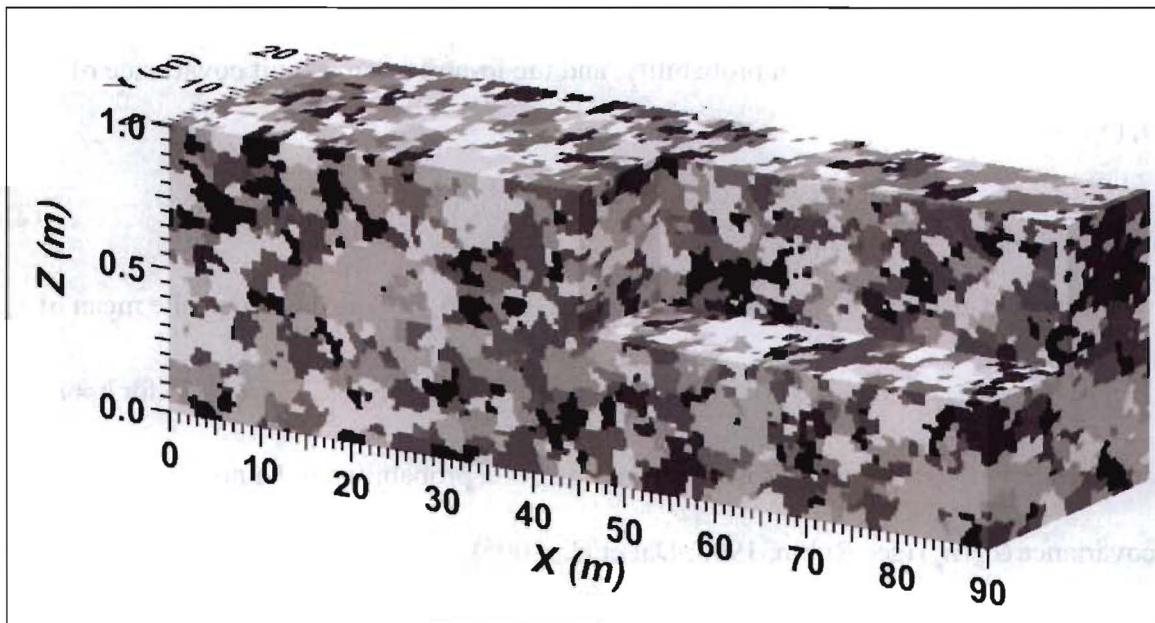


Figure 1. An example of the multi-facies sediments created with indicator Kriging model

2. Conductivity covariance function in multi-faces heterogeneous sediments

Let $Y(\mathbf{x})$ be the spatial random function of log-conductivity, which can be divided into subpopulations according to facies as per Rubin (1995),

$$Y(\mathbf{x}) = \sum_{k=1}^N I_k(\mathbf{x}) Y_k(\mathbf{x}), \quad (1)$$

where $Y_k(\mathbf{x})$ represents log-conductivity within facies k . According to Dai et al. (2004) and Ritzi et al. (2004), the composite covariance $C_Y(\mathbf{h}_\phi)$ of $Y(\mathbf{x})$ can be represented in terms of proportion, transition probability, and the in-unit or cross-unit covariance of $Y_k(\mathbf{x})$ as

$$C_Y(\mathbf{h}_\phi) = \sum_{k=1}^N \sum_{i=1}^N \{C_{ki}(\mathbf{h}_\phi) + m_k m_i\} p_k t_{ki}(\mathbf{h}_\phi) - M_Y^2, \quad (2)$$

where m_k and σ_k^2 denote the mean and variance of $Y_k(\mathbf{x})$; M_Y is the composite mean of $Y(\mathbf{x})$. It is assumed that the cross-covariances are negligible, i.e., $C_{ki}(\mathbf{h}_\phi) = 0$ for $k \neq i$, and we apply the exponential functions for transition probability and auto-covariance $C_{kk}(\mathbf{h}_\phi)$ (see Rubin, 1995; Dai et al., 2005),

$$t_{ki}(\mathbf{h}_\phi) = p_i + (\delta_{ki} - p_i) e^{-\frac{h_\phi}{\lambda_i}} \quad (k, i = \overline{1, N}), \quad (3a)$$

$$C_{kk}(\mathbf{h}_\phi) = \sigma_k^2 e^{-\frac{h_\phi}{\lambda_k}} \quad (k = \overline{1, N}), \quad (3b)$$

Where σ_k^2 and λ_k are variance of log conductivity and integral scale of k facies, and λ_i is the indicator correlation length. Finally, we obtain the composite covariance function as

$$C_Y(\mathbf{h}_\phi) = \sum_{k=1}^N p_k^2 \sigma_k^2 e^{-\frac{h_\phi}{\lambda_k}} + \sum_{k=1}^N p_k (1 - p_k) \sigma_k^2 e^{-\frac{h_\phi}{\lambda_k}} + \frac{1}{2} \sum_{k=1}^N \sum_{i=1}^N (m_k - m_i)^2 p_k p_i e^{-\frac{h_\phi}{\lambda_i}}, \quad (4)$$

where $\lambda_\psi = \lambda_k \lambda_l / (\lambda_k + \lambda_l)$ and λ_k is the integral scale of log conductivity in facies k .

3. Macrodispersivity equations

To derive the macrodispersivity equations, we use the same assumptions as Rubin (1995): (1) the flow field is at steady state, (2) the conductivity field is weakly stationary, (3) the velocity field is uniform in the mean, (4) the flow domain is unbounded, and (5) the variance of the log conductivity is smaller than unity. Furthermore, assuming that the mean displacement velocity of a solute particle is approximated at the first order by the average fluid velocity, the macrodispersion coefficients are computed by:

$$D_{jl}(t) = \int_0^t u_{jl}(U_1 t') dt' \quad (5a)$$

$$\hat{u}_{jl}(\mathbf{k}) = U_1^2 \left(\delta_{lj} - \frac{k_j k_l}{k^2} \right) \left(\delta_{ll} - \frac{k_l k_l}{k^2} \right) \hat{C}_Y(\mathbf{k}) \quad (j, l = 1, \dots, d) \quad (5b)$$

where $D_{jl}(t)$ is the macroscopic dispersivity tensor, u_{jl} is the velocity covariance, the circumflex denotes the Fourier transform operator and U_1 is the mean velocity. Following Rubin (1995) and replacing the bimodal covariance function with the multimodal covariance of Equation (4), we derived the longitudinal and transverse macrodispersion coefficients in the three-dimensional domain as

$$\frac{D_{11}(t)}{U_1} = \sum_{k=1}^N \sigma_k^2 p_k \left(p_k \lambda_k A(\tau_1) + (1-p_k) \lambda_\psi A(\tau_2) + \frac{\lambda_l}{2\sigma_k^2} A(\tau_3) \sum_{i=1}^N p_i (m_k - m_i)^2 \right), \quad (6)$$

$$\frac{D_{22}(t)}{U_1} = \sum_{k=1}^N \sigma_k^2 p_k \left(p_k \lambda_k B(\tau_1) + (1-p_k) \lambda_\psi B(\tau_2) + \frac{\lambda_l}{2\sigma_k^2} B(\tau_3) \sum_{i=1}^N p_i (m_k - m_i)^2 \right), \quad (7)$$

where, $A(\tau_i) = 1 + \frac{4}{e^\tau \tau_i^4} \left[6(e^{\tau_i} - \tau_i - 1) - \tau_i^2(e^{\tau_i} + 2) \right]$, τ_i is the dimensionless time expressed

as $\tau_1 = tU_1/\lambda_k$, $\tau_2 = tU_1/\lambda_\nu$, $\tau_3 = tU_1/\lambda_l$,

and $B(\tau_i) = \frac{1}{e^\tau \tau_i^4} \left[12(1 + \tau_i - e^{\tau_i}) + \tau_i^2(5 + e^{\tau_i} + \tau_i) \right]$.

Equations (6) and (7) relate the macrodispersion coefficients to the facies statistical parameters such as the facies proportion and correlation length, and the variance and mean of log conductivity. The macrodispersion coefficients are positively correlated with the mean difference (or the contrast) of log conductivity. Figure 2 shows the macrodispersion coefficients increase with the increasing conductivity contrast, which is defined as $\rho = \bar{K}_{\max}/\bar{K}_{\min}$, where \bar{K}_{\max} and \bar{K}_{\min} are the maximum and minimum geometric means of conductivity within the N facies ($\bar{K}_i = e^{m_i}$, $i = \overline{1, N}$). When $\rho = 1$, the third term (also called the cross-facies-transition term) in (6) and (7) is zero and the macrodispersion coefficients only consist of the first two terms (also called the auto-transition terms or within-facies-transition). When ρ increases, the contribution of the cross-transition term to the macrodispersion increases. When $\rho \geq 10$, the cross-transition term dominates over the auto-transition terms. The results in Figure 2 indicate that the variation of conductivity within and across facies is the source of the macrodispersion and in a homogeneous aquifer system the macrodispersion coefficients are zero.

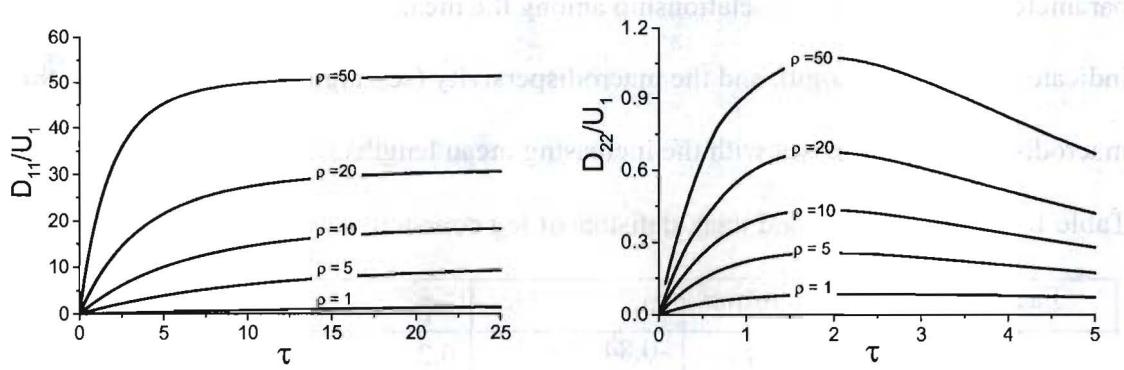


Figure 2. Sensitivity of the longitudinal and transverse macrodispersion coefficients to conductivity contrast ($\rho = \bar{K}_{\max} / \bar{K}_{\min}$) in the three-dimensional domain ($\tau = U_1 t / \lambda_I$).

When time is sufficiently large, the transverse macrodispersivity approaches zero, while the longitudinal macrodispersivity has the following simplified expression,

$$\frac{D_{11}}{U_1} = \sum_{k=1}^N \sigma_k^2 p_k \left(p_k \lambda_k + (1 - p_k) \lambda_\psi + \frac{\lambda_I}{2\sigma_k^2} \sum_{i=1}^N p_i (m_k - m_i)^2 \right). \quad (8)$$

Equation (8) shows how different modes of variability in log conductivity contribute to the macrodispersion at the later time. For a unimodal distribution of facies, $N = 1$, Equation (8) becomes $D_{11}/U_1 = \sigma^2 \lambda$, which is the same as the unimodal macrodispersivity derived by Dagan (1989) and Gelhar (1993). Equation (8) provides a way to estimate the longitudinal macrodispersivity of a multimodal conductivity field from the facies proportions, mean and variance of log conductivity in each facies, and the indicator correlation length.

In order to analyze the impact of facies mean lengths on macrodispersion with equation (8), we create a set of synthetic data of log conductivity (Table 1), and use them to estimate the longitudinal macrodispersion coefficients with variable mean length of the floodplain. When we vary the mean length of floodplain from 1 to 30 m and fix other

parameters, we find a linear relationship among the mean length of the floodplain, the indicator correlation length, and the macrodispersivity (see Figure 3), which means the macrodispersivity increases with the increasing mean lengths of the facies.

Table 1. Sediment facies and their statistics of log conductivity

Facies	k	Proportion	m_k	σ_k^2	λ_k
Sand	1	0.07	-0.84	0.2	0.9
Silt sand	2	0.56	-3.14	0.5	1.0
Fine sand	3	0.19	-1.76	0.3	1.2
Coarse sand	4	0.18	1.46	0.55	1.1

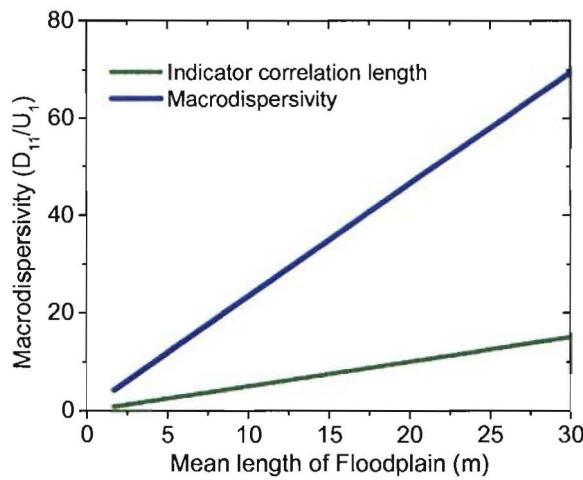


Figure 3. Facies mean length vs. indicator correlation length and macrodispersivity.

4. Conclusions

The composite covariance function of multi-modal log conductivity for heterogeneous sediments allows us to derive the associated macrodispersion coefficients for solute transport in a three-dimensional domain. This, in turn, facilitates analyzing the link between aquifer architecture and plume spreading. We can easily and independently

analyze the relative contributions of facies proportions, mean lengths, in-facies variance and per-facies co-variance in log-conductivity, and the difference in mean log-conductivity across facies. At late time, the longitudinal dispersivity coefficient clearly shows a linear dependence on the variance of log conductivity, the mean length of facies and the indicator correlation length.

Acknowledgements: This work was supported by the National Science Foundation under grant NSF-EAR 00-01125. Any opinions, findings and conclusions or recommendations expressed in this paper are those of the authors and do not necessarily reflect those of the National Science Foundation.

References

Dagan, G., *Flow and transport in porous formations*, Springer-Verlag, New York, 465 p, 1989.

Dai, Z., R. W. Ritzi, C. Huang, D. F. Dominic, and Y. N. Rubin, Transport in heterogeneous sediments with multimodal conductivity and hierarchical organization across scales, *J. Hydrol.*, 294, 68–86, 2004.

Dai, Z., R. W. Ritzi, and D. F. Dominic, Improving permeability semivariograms with transition probability models of hierarchical sedimentary architecture derived from outcrop-analog studies, *Water Resour. Res.*, 41, W07032, doi:10.1029/2004WR003515, 2005.

Dai, Z., A. Wolfsberg, Z. Lu, and P. Reimus, Upscaling matrix diffusion coefficients for heterogeneous fractured rocks, *Geophys. Res. Lett.*, 34, L07408, doi:10.1029/2007GL029332, 2007.

Gelhar, L.W., 1993. Stochastic Subsurface Hydrology, Prentice-Hall, Englewood Cliffs, NJ.

Lu, Z. and D. Zhang, On stochastic modeling of flow in multimodal heterogeneous formations, *Water Resour. Res.*, 38(10), 1190, doi: 10.1029/2001WR001026, 2002.

Ritzi, R. W., Z. Dai, D. F. Dominic, and Y. N. Rubin, Spatial correlation of permeability in cross-stratified sediment with hierarchical architecture, *Water Resour. Res.*, 40, W03513, doi:10.1029/2003WR002420, 2004.

Rubin, Y., Flow and transport in bimodal heterogeneous formations, *Water Resour. Res.*, 31(10), p. 2461-1468, 1995.

Rubin, Y., *Applied Stochastic Hydrogeology*, Oxford Press, 2003.

Zhang, D., *Stochastic Methods for Flow in Porous Media: Coping With Uncertainties*, 350pp., Academic, San Diego, Calif., 2002.