On the influence of higher moments to tracer transport in heterogeneous porous media

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1. Abstract

Flow and transport processes are mainly characterized by multi-scale physical interpretation, variability and heterogeneity of all variables, such as hydraulic conductivity or sorption. The only rational way for describing uncertainties is by using stochastic modeling. Heterogeneity is usually described by variogram or multi-Gaussian (MG) field which is not able to reproduce curvilinear high or low connected *lnK* zones. Moreover, many analytical first-order solutions have been obtained, but they are limited by uniform and steady mean flow, low heterogeneity and also rely only on two first statistical moments. On the other side, field observations show that describing solute and flow variables with only two moments, mean and variance, insufficiently describes specified physical processes implying predefined Gaussianity. Using Adaptive Fup Monte-Carlo Method (AFMCM), we analyze travel time statistics for different *lnK* variability, MG and non-Gaussian heterogeneity fields, in uniform and radial convergent computational setup. Higher moments are needed for accurate description of early and late arrivals, as well as travel time peak, in case of highly heterogeneous MG fields and especially non-Gaussian fields with connected highly permeable *lnK* zones. Involving local diffusion and using Random Walk Particle Tracking Method (RWPT) over continuous velocity field, normalized concentration pdf is obtained with respect to Maximum Entropy (MaxEnt) and beta pdf. Even in mild heterogeneous aquifers, concentration pdf is not completely described by first two moments. MaxEnt pdf requires more than four moments for accurate description, however beta pdf presents relatively well matching with simulated Monte-Carlo pdf.

2. Methodology and Computational Setup

Adaptive Fup Monte-Carlo Method (AFMCM)
[*Gotovac et al.* 2009a]

Heterogeneity
- Generation of $Y = lnK$ realizations [HYDROGEN, *Bellin and Rubin*, 1996]
- Transformation of lnK fields in Fup basis using the Fup Collocation Transformation – FCT [*Gotovac et al.*, 2009a]
- Generation of non-Gaussian fields [*Zinn and Harvey*, 2003]

Flow in Heterogeneous Porous Media
- Darcy law:

$$v_i = \frac{q_i}{n} = -\frac{K}{n}\frac{\partial h}{\partial x_i} \quad ; i = x,y$$

- Flow equation:

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} + \frac{\partial Y}{\partial x}\frac{\partial h}{\partial x} + \frac{\partial Y}{\partial y}\frac{\partial h}{\partial y} = Q$$

- Adaptive Fup Collocation Method (AFCM) - continuous head and velocity fields [*Gotovac et al.*, 2009a]

Contaminant Transport
- Random Walk Particle Tracking (RWPT):

$$X_{t+\Delta t} = X_t + \left[v_x(x_t,y_t) + \frac{\partial Dxx}{\partial x} + \frac{\partial Dxy}{\partial y}\right]\Delta t + \sqrt{2D_{xx}\Delta t}\,z_1 + \sqrt{2D_{xy}\Delta t}\,z_2$$

$$Y_{t+\Delta t} = Y_t + \left[v_y(x_t,y_t) + \frac{\partial Dyx}{\partial x} + \frac{\partial Dyy}{\partial y}\right]\Delta t + \sqrt{2D_{yx}\Delta t}\,z_1 + \sqrt{2D_{yy}\Delta t}\,z_2$$

- Continuous dispersion tensor form

$$D_{ij} = \alpha_T|\vec{v}|\delta_{ij} + (\alpha_L - \alpha_T)\frac{v_i v_j}{|\vec{v}|} + D^*\tau_{ij} \quad ; i,j = x,y$$

- In flux and Resident injection mode
- Resident concentration:

$$C_r(\vec{x},t) = \frac{\sum \Delta M_i \cdot m}{V_s}$$

- Flux-averaged concentration:

$$C_f(\vec{x},t) = \frac{q_x}{v}$$

- Travel time:

$$\tau(x) = \int_{x_0}^{x} \frac{1}{v[X_E(\xi), Y_E(\xi)]}d\xi$$

Monte-Carlo Statistics

- CDF:

$$F_\tau(t;x) = E(H(t-\tau(x))) = \frac{1}{N_P n_{MC}}\sum_{i=1}^{N_{MC}}\sum_{j=1}^{N_P}(H(t-\tau(x)))$$

- PDF:

$$f_\tau(t;x) = \frac{\partial(F_\tau(t;x))}{\partial t}$$

- MaxEnt Algorithm:
  - Shannon Entropy

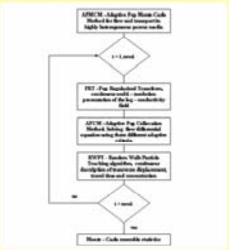
$$S(f) = -\int_{x_{min}}^{x_{max}} \ln(f(x))f(x)dx$$

  - The optimal MaxEnt Fup PDF approximation

$$f^*(x) = \exp\left(-1 - \sum_{j=0}^{N}\gamma_j Fup_{2,j}(x)\right)$$

  - MaxEnt Fup moments

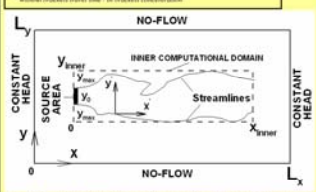
$$m_i = \int_0^1 x^i f^*(x)dx = \sum_{j=0}^{m} d_{ij}\int_0^1 Fup_{2,j}(x)f^*(x)dx + \int_0^1 \varepsilon_i(x)f^*(x)dx$$



Uniform Flow Setup
- Flow domain 64 x 32 I_Y
- multi-Gaussian field, non-Gaussian fields (DN,CN)
- Var(lnK) = 1 and 8
- Inner domain 40 x 26 I_Y
- $N_{PARTICLES}$ = 4000 (16000) *
- $n_{Monte\text{-}Carlo\ realizations}$ = 500 (1000) *
- y_0/I_Y = 12 ; in flux (resident) * injection mode

* without brackets travel time / in brackets concentration

Radial flow Setup
- Flow domain (64 x 64 I_Y)
- multi-Gaussian field, non-Gaussian fields (DN,CN)
- Var(lnK) = 1 and 8
- $N_{PARTICLES}$ = 4000
- $n_{Monte\text{-}Carlo\ realizations}$ = 500
- resident injection mode



Radial convergent flow

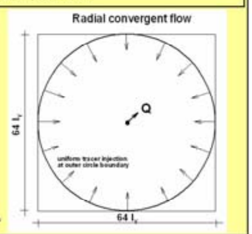


Figure 1. Simulation domain needed uniform mean flow (left) and radial convergent flow (right).

3. Heterogeneity

Due to usual scarcity of data, heterogeneity can be simply presented only with few parameters (mean, variance and correlation length) implying usage of common geostatistical kriging or "variogram based" techniques. This leads to estimation of only first two *lnK* statistical moments with respect to available data and application to so called classical "multi-Gaussian" heterogeneity structure [*Duetsch and Journel*, 1998; *Kitanidis*, 1997]. However, heterogenity cannot be uniquely presented by knowing only the histogram and variogram and additional information in terms of higher-order statistics are needed. Take for example the well-known and popular sequential Gaussian simulation (sGs) algorithm. Most users are aware that only a variogram and histogram model are needed for this conditional simulation method to work. Nevertheless, hidden in the algorithm is the strong assumption that everywhere in the reservoir the higher-order/multiple-point statistics are multivariate-Gaussian. It means that amongst all possible reservoir models that reproduce a given variogram model, sGs generates models that are maximally disconnected in the low and high values ("maximum entropy" property). It is therefore troubling to observe that a large majority of reservoir models built today are based on assumptions that carry little geological relevance. Moreover, variogram geostatistics is unable to describe curvilinear shapes of connected low/high pathways which are essentially important for reproducing the flow and transport processes in porous media. We generated three types of conductivity fields according to the procedure of *Zinn and Harvey* [2003]: (1) a standard MG field using the program Hydrogen [*Bellin and Rubin*, 1996]; Figure 2a, (2) a field with disconnected high conductivity, but connected patterns of low conductivity (disconnected field-DN); Figure 2b; and (3) a field with connected patterns of high conductivity (connected field-CN); Figure 2c. All three conductivity fields share the same basic statistics, the first and second statistical moments, but their higher lnK moments and therefore *lnK* structures differ in how the high and low values are connected.

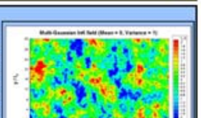


Figure 2a. Multi-Gaussian (MG) field

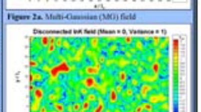


Figure 2b. DisconNected (DN) lnK field

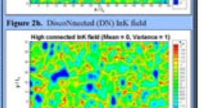


Figure 2c. CoNnected (CN) lnK field

4. Travel time statistics

The travel time pdfs for uniform flow and advective transport are illustrated on a log-log plot (Figure 3a-f) for the in flux injection mode and Var(lnK) values of 1 and 8 including all three fields. Figure 3 actually presents the Monte-Carlo experimental AFMCM pdf as well as its MaxEnt approximation pdf which uses the travel time moments up to the 6-th order. Figure 4a-b presents results for MG fields with Gaussian variogram. In summary, deviations from a symmetrical distribution (e.g., log-normal, very close to ADE model, see *Gotovac et al.*, 2009b) or from MaxEnt pdf with the first two moments decrease with distance from the source, and increase significantly with increasing Var(lnK). For low and mild heterogeneity (Figure 3a), small deviations from a symmetric distribution occur only within the first 10-20 integral scales, while higher travel time moments only slightly influenced the pdf close to the source area and mean and variance completely describe advective transport in MG field. For high heterogeneity (Figure 3b), the computed AFMCM pdf is increasingly asymmetric; the main influence is presented by the third moment, which quantifies the pdf skewness. Figure 4c-d presents pdf results for CN (connected) fields that are characterized by thin curvilinear layers of connected high lnK values which play a dominant role in transport subsurface processes. Connected lnK layers create preferential flow channels that reduce travel time and significantly change travel time pdf or tracer breakthrough curve. Figure 3c shows that 'channeling' effect also depends on heterogeneity level because low heterogeneity exhibits pdf completely described only by two travel time moments. However, it is a not case for high heterogeneity (Figure 3d) where channeling effect is completely developed. In the CN travel time pdf, the most important influence is given by kurtosis rather than skewness as in the MG fields. The fourth moment completely describes peak and late arrivals. Due to faster early arrivals, higher peak and fatter late tailings travel time pdf is more skewed and significantly changed. It implies that MaxEnt pdf or tracer breakthrough model needs to use four parameters in order to completely reproduce actual pdf in the CN field. Figure 3e-f presents pdf results for DN (disconnected) fields that are characterized by low correlation of high lnK values, but significant correlation of connected low lnK zones. Results show that connectedness of low lnK zones drastically affects travel time pdf so that pdf is symmetric and can be fully described by first two travel time moments and consequently classical ADE model, even for high heterogeneity.

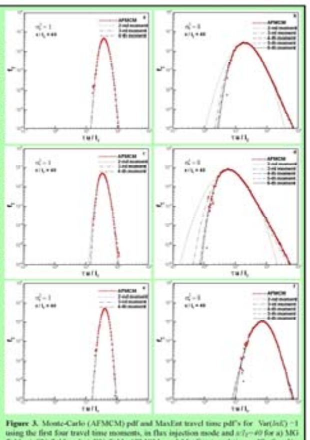


Figure 3. Monte-Carlo (AFMCM) pdf and MaxEnt travel time pdf's for Var(lnK) =1 using the first four travel time moments, in flux injection mode and x/I_Y=40 for a) MG field, c) CN field and e) DN field. AFMCM and MaxEnt travel time pdf's for Var(lnK)=8 using the first six travel time moments, in flux injection mode and x/I_Y=40 for b) MG field, d) CN field and f) DN field.

The travel time pdf-s for radial flow and advective transport are illustrated on a log-log plot (Figure 4a-c) for the resident injection mode and Var(lnK) value of 8 including all three fields. Again, log-normal distribution does not describe all pdf features, especially early arrivals for all three fields. Skewness is the most important moment for peak and late arrivals in MG and CN fields. Late arrivals are also subjected to the power law as in the uniform flow case. There is no anomalous transport in all three fields because slopes of the late arrivals for both setup cases are always higher than 2:1 [*Berkowitz and Scher*, 1995]. According to the [*Zuber and Kreft*, 1978] relationship between travel time variance and mean can yield longitudinal macrodispersivity. The first order theory yields a well-known relation which is appropriate for MG field and low heterogeneity. Figure 5 suggests that our results confirm findings of *Wen and Gomez-Hernandez* [1998] and *Zinn and Harvey* [2003] that macrodispersivity is significantly larger in CN fields than in the classical MG field, even for a low heterogeneity. Opposite behavior is visible for DN fields. For instance, macrodispersivity is 12% greater for CN field and 30% smaller for DN field and low heterogeneity, while macrodispersivity is around three times greater for CN field and around three times smaller for DN field and high heterogeneity.

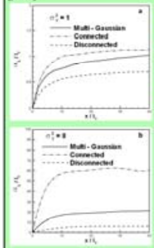


Figure 5. Longitudinal dispersivity for Var(lnK) 1 and 8 including all fields

Figure 4. Monte-Carlo (AFMCM) pdf and MaxEnt travel time pdf's for Var(lnK) = 8 for radial convergent flow using the first three travel time moments, resident injection mode and r/I_Y=32 for a) MG field, b) CN field and c) DN field.

5. Concentration statistics

Concentration Monte-Carlo statistics for multi-Gaussian field (Var(lnK)=1) is presented sequentially in Figures 6a –6d. Figure 6a presents the first statistical moment in snapshot over the whole inner domain for dimensionless time τ = 10, with peak located in plume center. Variance (Fig. 6b) is similar like mean with the same peak position. In Figure 6c skewness takes values around 3 near the plume center. Skewness increases its values as the distance from the plume center increases. Kurtosis (Fig 6d) is in functional relationship with skewness presented with $K = 1 + S^2$. As could be seen, uncertainty is highest at boundary plume areas suggesting a importance of higher concentration moments. This is presented in Figure 7, where MaxEnt pdf requires more than two moments for approximation of simulated MC pdf. The MaxEnt pdf with four and six moments, is still not enough for accurate matching with MC pdf. On the other side, beta pdf matches fairly well MC pdf, except in area close to zero concentration. Since beta pdf is two parametric one, it suggests that higher order concentration moments relatively accurate could be approximated with first two moments. Finally, future simulations will show concentration pdf behavior in highly heterogeneous porous media.

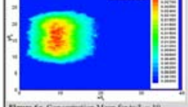


Figure 6a. Concentration Mean for tu/I_Y= 10

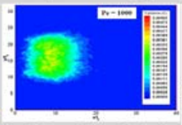


Figure 6b. Concentration Variance for tu/I_Y= 10

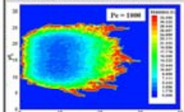


Figure 6c. Concentration Skewness for tu/I_Y= 10

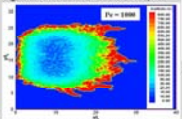


Figure 6d. Concentration Kurtosis for tu/I_Y= 10

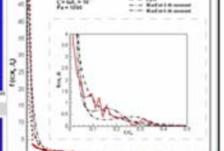


Figure 7. Concentration pdf for tu/I_Y= 10 and Pe = 1000

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