INSTITUT P'

Monte Carlo analysis of macro dispersion in 3D heterogeneous porous media

Arthur Dartois and Anthony Beaudoin

Institute P', University of Poitiers, France

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UNIVERSITAS STUDIORUM ZAGRABIENSIS MDCLXIX

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Introduction

The transport of solute in geological media is a key phenomena in a lot of applications.

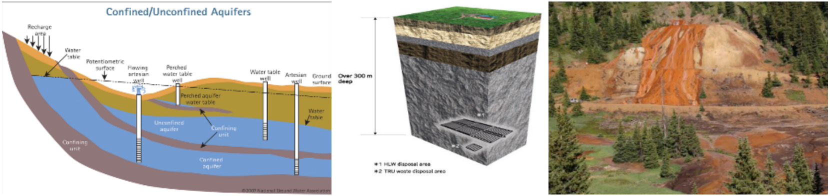

Figure 1 : Examples of applications, freshwater supply (left), geological waste disposal (middle) and remediation of mine drainage (right).

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Heterogeneous porous media

Random permeability field:

Lognormale distribution	$Y = log(K)$
Correlation function	$C_y(r) = \sigma_y^2 exp(-\|r\|\lambda_y)$

where σ^2 is the lognormal permeability variance, $|r|$ is the distance between two points and λ is the correlation length.

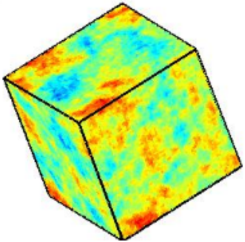

Figure 2 : Permeability field

Generation of random permeability field [G. 1989; Gelhar and al. 1993]
Fourier transform method using the parallel library FFTW [Frigo and al. 2005; Gutjahr and al. 1989]

Heterogeneous porous media

Saturated flow:

flow equation	$\nabla(K\nabla h) = 0$
Boundary conditions	• fixed head on two opposite borders • periodic boundary conditions on the other transverse faces
Darcy's law	$v = -K/\theta\nabla h$

Finite volume scheme [Chavent and al. 1991]
Parallel multi grid solver HYPRE [Falgout and al. 2005]

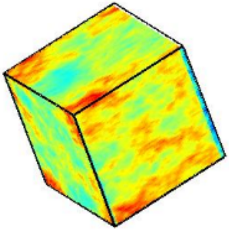

Figure 3 : Flow field

Particles transport

Transport equation:

$$\frac{\partial \theta C}{\partial t} + \nabla \cdot (\theta C v) - \nabla \cdot (\theta D \nabla C) = 0$$

$$D_{ij} = (\alpha_T |v| + D_m)\delta_{ij} + \frac{(\alpha_L - \alpha_T)\, v_i v_j}{|v|}$$

where α_L and α_T are the longitudinal and transverse dispersivities and D_m is the molecular diffusion coefficient.

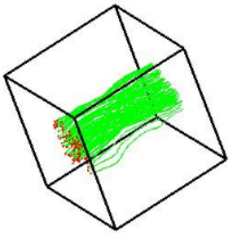

Figure 4 : Particles paths

Random walk method [Kampen and al. 1981].
Discretization using a stochastic RK method of strong order 1.5 [Burrage and Burrage 1996].
An adaptative time step depending of the maximum velocity.

Peclet related to the hydrodynamic dispersion: $Pe_L = \lambda/\alpha_L$
Peclet related to the molecular diffusion: $Pe = \lambda u/D_m$

Macro dispersions:

$$D_L^i(t) = \frac{1}{2\lambda u}\frac{d\left(\langle x^2(t)\rangle_i - \langle x(t)\rangle_i^2\right)}{dt}$$

$$D_T^i(t) = \frac{1}{2\lambda u}\frac{d\left(\langle y^2(t)\rangle_i - \langle y(t)\rangle_i^2\right)}{dt}$$

where $\langle x^k(t)\rangle_i$ and $\langle y^k(t)\rangle_i$ are the kth moments of the solute plume of the ith simulation.

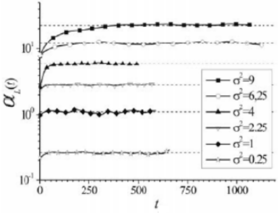

Figure 5 : Macro dispersion as function of time

The average over N_S Monte Carlo simulations is performed in a second step:

$$D_L(t) = \langle D_L^i(t)\rangle_{i=1,N_S} \quad \text{and} \quad D_T(t) = \langle D_T^i(t)\rangle_{i=1,N_S}$$

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Diffusion and local dispersion in 2D

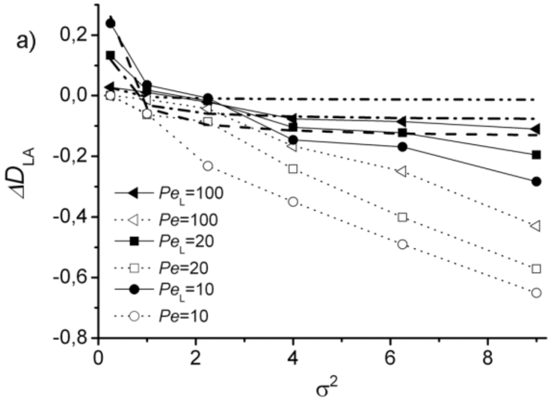

Figure 6 : Relative difference of longitudinal macro dispersion as function of σ_y^2 for various values of Pe and Pe_L.

[Dreuzy, Beaudoin, and Erhel 2007; Beaudoin, Dreuzy, and Erhel 2010]

Diffusion and local dispersion in 2D

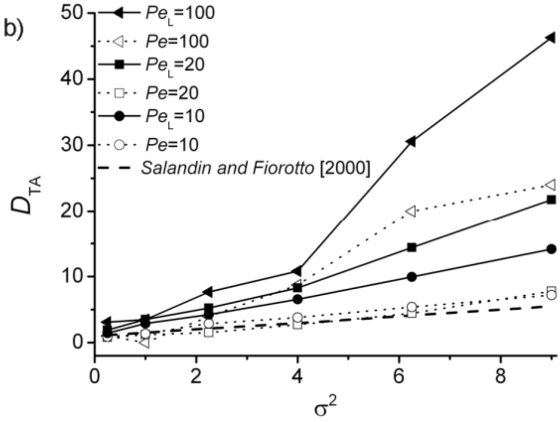

Figure 7 : Transverse macro dispersion as function of σ^2 for various values of *Pe* and Pe_L.

[Dreuzy, Beaudoin, and Erhel 2007; Beaudoin, Dreuzy, and Erhel 2010]

Diffusion and local dispersion in 2D

In conclusion in 2D:

- Diffusion induces a reduction of the longitudinal macro dispersion coefficient twice as large as local dispersion.
- Dispersion due to permeability heterogeneities amplifies the transverse macro dispersion coefficient 1.5-3 times as much as diffusion.

It's explain by the fact that the local dispersion is larger than diffusion in the high velocity zones whereas diffusion is larger than the local dispersion in the low velocity zones.

Advection only in 3D

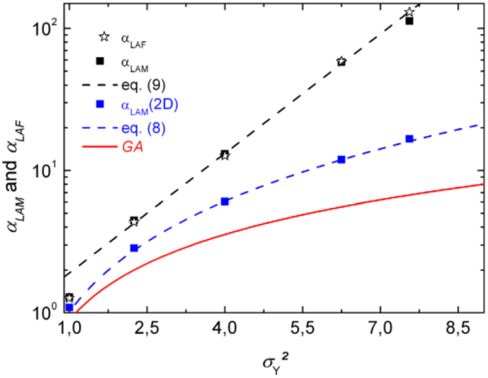

Figure 8 : Longitudinal macro dispersion estimated by fitting the time dependent dispersivities α_{LAF} and by its long-time averaging α_{LAM} as function of σ^2.

The longitudinal macrodispersivity is compared to the value obtained numerically in 2D (blue squares) and to the perturbative approximation [Gelhar and al. 1983] (red line).

Advection only in 3D

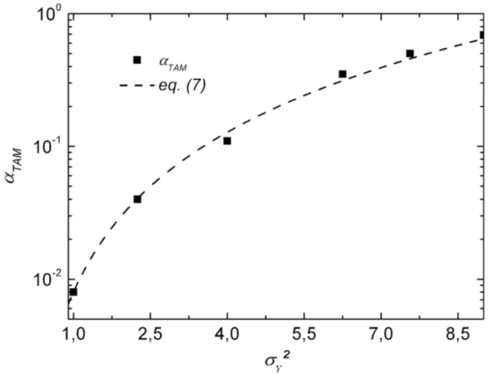

Figure 9 : Transverse macro dispersion estimated by its long-time averaging α_{TAM} as function of σ_y^2.

[Dreuzy, Beaudoin, and Erhel 2007; Beaudoin and Dreuzy 2013]

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Visualisation

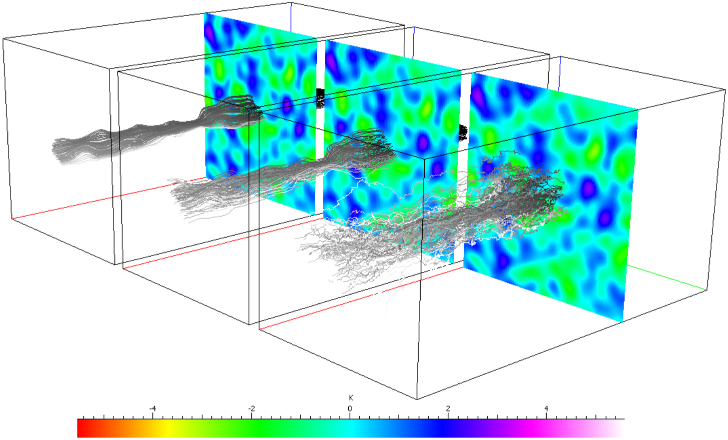

Figure 10 : Particles paths in a permeability field with $\sigma^2 = 1$ and several value of Peclet (from left to right: $Pe = 1000$, $Pe = 100$, $Pe = 10$).

Visualisation

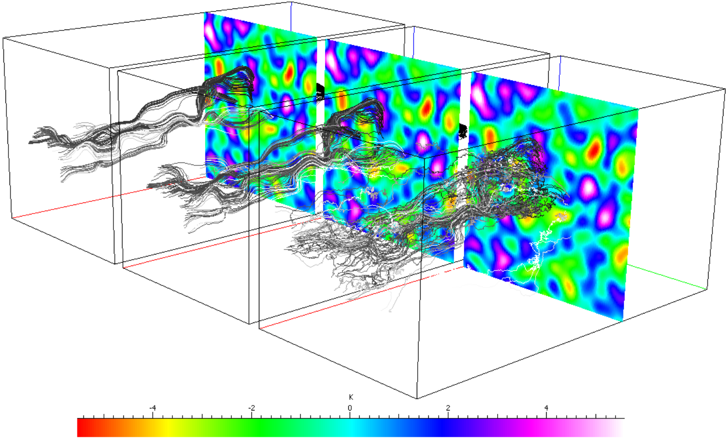

Figure 11 : Particles paths in a permeability field with $\sigma^2 = 4$ and several value of Peclet (from left to right: $Pe = 1000$, $Pe = 100$, $Pe = 10$).

Visualisation

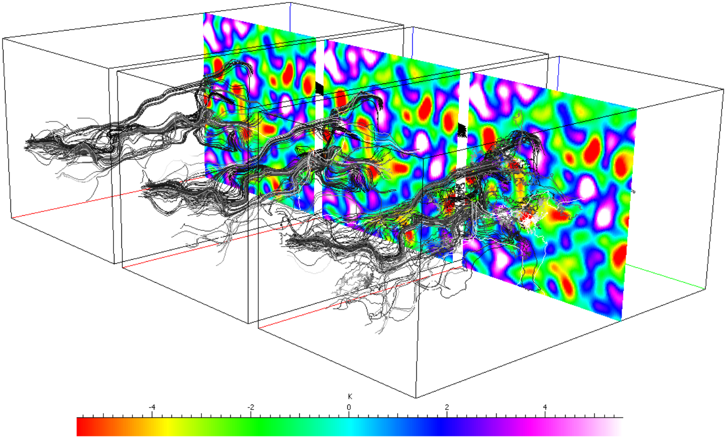

Figure 12 : Particles paths in a permeability field with $\sigma^2 = 9$ and several value of Peclet (from left to right: $Pe = 1000$, $Pe = 100$, $Pe = 10$).

Longitudinal Macro dispersion

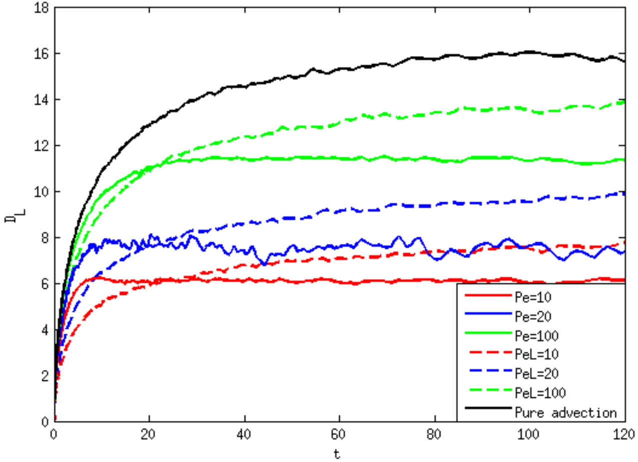

Figure 13 : Longitudinal macro dispersion D_L as a function of time for several value of Pe and Pe_L for $\sigma^2 = 4$.

Transversal Macro dispersion

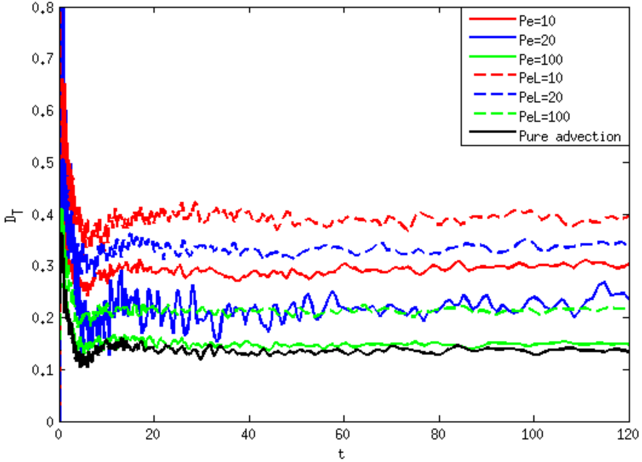

Figure 14 : Transverse macro dispersion D_T as a function of time for several value of Pe and Pe_L for $\sigma^2 = 4$.

Longitudinal macro dispersion

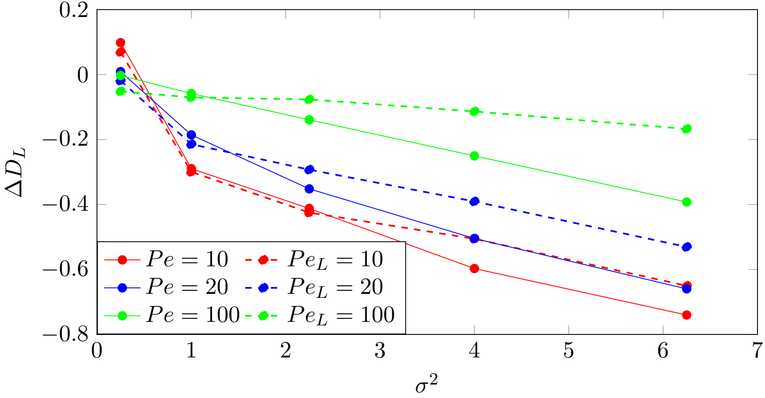

Figure 15 : Relative difference of longitudinal macro dispersion ΔD_L as a function of σ^2 for different value of Pe and Pe_L.

Transversal macro dispersion

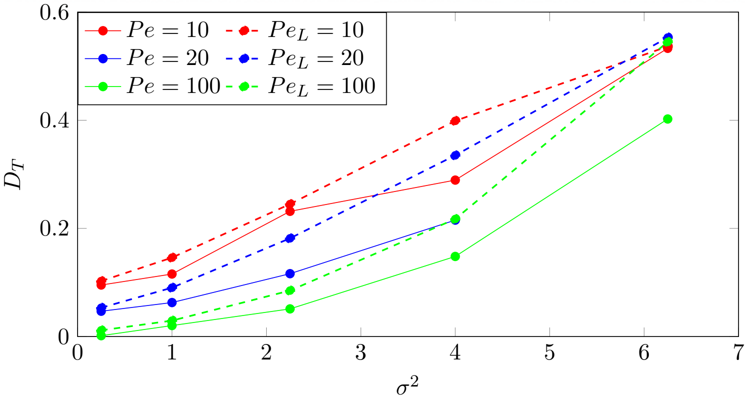

Figure 16 : Transversal macro dispersion as a function of σ^2 for different values of Pe and Pe_L.

Macro dispersion conclusions

For the longitudinal macro dispersion:

- The effect of diffusion and local dispersion is stronger in 3D than in 2D.
- The difference between the impact of diffusion and local dispersion is smaller in 3D

For the transverse macro dispersion:

- We have a positive impact on the transerve macro dispersion from the diffusion and the local dispersion
- The local dispersion still has also a stronger impact on the transerve macro dispersion than the diffusion
- The amplification observe from the heterogeneity in 2D is almost non-existent in 3D

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Conclusions and outlooks

Conclusions:

• We have almost completed the study of the impact of molecular diffusion and local dispersion on the macro dispersion in 3D.

• We haven't been able yet to compute the asymptotic value of the macro dispersion for $\sigma^2 = 9$.

Outlooks:

• We are currently working on visualisations methods to increase our understanding of these phenomena (implementation of .vtk output).

• The next step will be the implementation of chemical reaction between particles.

• We are also investigating a new method of particles transport which should reduce the computations times by an huge factor.

Thank you for your attention!

Bibliography I

A. Beaudoin and J.-R. de Dreuzy. "Numerical assessment of 3D macrodispersion in heterogeneous porous media". In: *Water Ressources Research* 43 (2013).

A. Beaudoin, J.-R. de Dreuzy, and J. Erhel. "Numerical Monte Carlo analysis of the influence of pore-scale dispersion on macrodispersion in 2D heterogeneous porous media". In: *Water Ressources Research* 46 (2010).

K. Burrage and P.M Burrage. "High strong order explicit Runge-Kutta methods for stochastic ordinary differential equations". In: *Applied Numerical Mathematics* 22 (1996).

Chavent and al. "A unified physical presentation of mixed, mixed-hybrid finite elements and standard finite difference approximations for the determination of velocities in waterflow problems". In: *Adv. Water Ressources* 14 (1991).

Bibliography II

J.-R. de Dreuzy, A. Beaudoin, and J. Erhel. “Asymptotic dispersion in 2D heterogeneous porous media determined by parallel numerical simulations”. In: *Water Ressources Research* 43 (2007).

Falgout and al. “Pursuing scalability for HYPRE’s conceptual interfaces”. In: *ACM Trans. Math. Software* 31 (2005).

Frigo and al. “The design and implementation of FFTW3”. In: *Proc. IEEE* 93 (2005).

Dagan G. “Flow and transport in porous formations”. In: *Springer Verlag* (1989).

Gelhar and al. “Stochastic subsurface hydrology”. In: *Engelwood Cliffs, New Jersey* (1993).

Gelhar and al. “Three dimensional stochastic analysis of macrodispersion in aquifers”. In: *Water Ressources Research* 19 (1983).

Bibliography III

Gutjahr and al. “Fast Fourier transforms for random field generation”. In: *New Mexico Tech project report* (1989).

Van Kampen and al. “Stochastic Processes in Physics and Chemistry”. In: *Elsevier Sci.* (1981).