Numerical Monte-Carlo analysis of the influence of pore-scale dispersion on macrodispersion in heterogeneous porous media

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Résumé :

La macro dispersion est le résultat de la diffusion moléculaire et des processus dispersifs. De l'échelle des pores à l'échelle de Darcy, la dispersion est modélisée par des dispersivités constantes. A des échelles supérieures, la dispersion est à la fois due à la dispersion locale et à l'hétérogénéité de l'écoulement. Dans ce travail, nous étudions l'influence relative de la dispersion locale et de l'hétérogénéité de la perméabilité sur la macro dispersion avec une diffusion moléculaire négligeable pour une large gamme de dispersivités et des fortes hétérogénéités de la perméabilité. Pour des faibles dispersivités, l'influence relative de la dispersion locale sur la macro dispersion est inférieure à 5% de la macro dispersion due uniquement à la perméabilité hétérogène. Pour des larges dispersivités, les effets de la dispersion locale sont limités à 25% de la macro dispersion due uniquement à l'hétérogénéité de la perméabilité.

Abstract :

Macrodispersion is the result of molecular diffusion and dispersion processes. From pore scale to Darcy scale, dispersion is commonly modeled by fixed longitudinal and transverse dispersivities. At larger scales, dispersion comes both from the smaller scale dispersion and from the heterogeneity of the flow. In this study, we investigate the relative influences of the pore-scale dispersion and of larger scale permeability heterogeneities on the macrodispersion when neglecting the molecular diffusion for a large range of dispersivities and permeability levels of heterogeneity. For smaller dispersivities, the relative influence of the pore-scale dispersion on the macrodispersion is smaller than 5% of the macrodispersion due only to permeability heterogeneities. For larger dispersivities, the effects of the local dispersion are limited to 25% at most of the macrodispersion due only to permeability heterogeneities.

Key words : Solute transport, macrodispersion, parallel computing, hydrodynamic dispersion.

1 Introduction

Dispersion results from the variations in fluid velocity occurring from the pore scale to the formation scale and from molecular diffusion [11]. It is modeled by an equivalent diffusion law parameterized by the dispersion tensor D [1]. This formalism is mostly used at two scales. At the local scale, the dispersion coefficient results from the effects of the variations of the pore-scale fluid velocity. At field scale, the dispersion coefficient also called macrodispersion comes both from the previous local effects and from the variations in fluid velocities due to permeability heterogeneities. In this study, we focus on the effects of the local dispersion on the macro-dispersion for highly heterogeneous 2D porous media. We take the most classical synthetic model of porous media. It consists in an exponentially correlated lognormal isotropic permeability field [9]. The originality of this work does not rely on the correlation structure but on the magnitude of the heterogeneity. We investigate the high heterogeneity cases while most previous studies dealt with the low heterogeneity cases [4, 12]. For low levels of heterogeneity and local dispersivities much smaller than the correlation length, the first-order perturbation analysis of *Gelhar and Axness* [1983] shows that the local dispersion does not modify the longitudinal macrodispersion D_{LA} and lets the transverse dispersion D_{TA} increase according to $D_{LA}/u=\lambda\sigma^2$ and $D_{TA}/u=\sigma^2/8(\alpha_L+3\alpha_T)$ where the index A stands for

asymptotic dispersion equivalent here to macrodispersion and u is the mean velocity. The longitudinal and transverse macrodispersions are proportional respectively to the correlation length λ and to the local dispersivities, α_L and α_T. When introducing non-ergodic conditions in the form of an injection window smaller than the correlation length, D_{LA} has been found to be reduced by no more than 10% for λ/α_L=20 [8]. Semi-analytical approaches accounting in the dispersion term for velocity variations confirm the low dependence of the longitudinal macrodispersion on σ^2 [16]. *Salandin and Fiorotto* [2000] show that the local dispersion induces an increase of both the longitudinal and transverse macrodispersions for σ^2<1. Differences with the solution of *Gelhar and Axness* [1983] are more important for the transverse component than for the longitudinal component of the macrodispersion. For high heterogeneity cases, *Salandin and Fiorotto* [2000] use their semi-analytical solution to predict a decrease of the longitudinal macrodispersion. They also give an estimate of the transverse macrodispersion. Still for σ^2>1, the sole numerical simulations have been performed for single realizations with α_L=0.15 m and α_T=0.015 m on a 2047 m by 511 m grid with 1 m by 1 m square grid cells [17]. For λ=2 m and 8 m corresponding respectively to $\lambda/\alpha_L\approx$13.5 and $\lambda/\alpha_L\approx$54, the normalized time-dependent dispersion $D_L(t)/(u\lambda\sigma^2)$ ranges between 1.2 and 1.4 in the first case and between 1 and 1.75 in the second case for $0.25<\sigma^2<4$. No conclusion can be drawn from the time-dependent transverse dispersion coefficient $D_T(t)$ because of its high variability due to the strong influence of local fluctuations in the velocity field. The main difficulty of numerical studies comes from the necessity to perform large scale and finely resolved Monte-Carlo simulations.

2 Model, numerical scheme and algorithms

In this paper, we use a basic non intrusive Monte-Carlo method. Lognormally and exponentially correlated permeability fields are generated with a Fourier transform method [13] using the parallel library FFTW [10]. The computation domains are regular square or rectangular grids of sizes L_x and L_y with square grid cells ($dx=dy=l_m$). The aspect ratio of the system L_x/L_y ranges from 1 to 2 from square to rectangular domains. The total number of grid cells varies between 2048 by 2048 and 16384 by 8192. The key characteristic scale is the permeability correlation length λ giving sense to the other scales. L_x/λ is the number of correlation length in the main flow direction taken here as x. λ/l_m is the grid cell resolution per correlation length. Ideally L_x/λ and λ/l_m should be both as large as possible. Flows follow the classical steady-state diffusion equation $\nabla(K\nabla h)=0$ with K the permeability and h the hydraulic head. Boundary conditions are like those on a permeameter with a fixed head on the vertical sides and no flow on the horizontal sides of the domain. The flow equations is discretized with a finite volume scheme and harmonic intermesh permeabilities [5]. The finite volume discretization yields a large-scale linear system solved with the algebraic multigrid implemented in HYPRE [2]. Velocity is first computed on each grid face and then derived within the grid cells from linear interpolations both in x and y directions as it is the sole interpolation scheme that verifies the continuity equation [14]. Solute transport follows the classical advection dispersion equation with the dispersion tensor given by equation. We assume a constant porosity. Injection is instantaneous on a large segment of length $I=0.4L_y$ perpendicular to the main flow direction and centered on the domain medium line. The segment is shifted downstream from the domain inlet by a distance of λ to avoid border effects. Injection is proportional to flow. Conditions are thus ergodic, meaning that the injection window is much larger than the correlation length as I/λ ranges from 80 to 320. The rate of advection to hydrodynamic dispersion is measured by the Peclet numbers, $Pe_L=\lambda/\alpha_L$ and $Pe_T=\lambda/\alpha_T$. We define also the Peclet number that characterizes the rate of advection to diffusion and is defined by $Pe=\lambda u/d$ with d the diffusion coefficient. Transport was simulated by a random walk particle tracking method fully described in several review papers [15]. We use the reflection method of *Uffink* [1985] to handle the discontinuities of the dispersion gradient. This choice is however not critical as it has been shown that dispersion results are not very sensitive to the method chosen for the lognormally and finitely correlated permeability fields even for σ^2 values as large as 4 [15]. Particles are injected according to flow in the injection window and are tracked using a parallel algorithm with synchronized communications of particles between cpus [3]. Our results rely on the effective dispersion coefficient [8]. The effective dispersion coefficient is obtained by averaging the dispersion coefficients obtained on a realization basis. The advantage of the effective dispersion is to avoid the dispersion of the mean solute plume positions between realizations. The longitudinal and transverse dispersion coefficients are first derived on a realization basis according to:

$$D^{i}_{L}(t) = 1/(2\lambda u)\ d(\langle x^2(t)\rangle_i - \langle x(t)\rangle^2_i)/dt \quad (1)$$

$$D^{i}_{T}(t) = 1/(2\alpha_T u)\ d(\langle y^2(t)\rangle_i - \langle y(t)\rangle^2_i)/dt \quad (2)$$

where $\langle x^k(t)\rangle_i$ and $\langle y^k(t)\rangle_i$ are the k^{th} moments of the solute plume of the i^{th} simulation. We underline that the longitudinal and transverse dispersion coefficients are normalized respectively by λu and $\alpha_T u$. These different normalization factors are deduced from the low heterogeneity approximations. In the absence of dispersion ($\alpha_L=\alpha_T=0$) but with diffusion ($d>0$), we normalize the transverse macrodispersion by the diffusion coefficient d. Equation 2 is replaced by:

$$D^{i}_{T}(t) = 1/(2d)\ d(\langle x^2(t)\rangle_i - \langle x(t)\rangle^2_i)/dt \quad (3)$$

The average over *Ns* Monte-Carlo simulations is performed in a second step:

$$D_L(t) = \langle D^{i}_{L}(t)\rangle_{i=1,Ns} \text{ and } D_T(t) = \langle D^{i}_{T}(t)\rangle_{i=1,Ns} \quad (4)$$

$\langle x^k(t)\rangle_i$ and $\langle y^k(t)\rangle_i$ are approximated from the random walkers position moments computed on realizations basis. All time-dependent dispersion results will be presented against t_N defined as the time t normalized by the characteristic time necessary to cross a correlation length λ ($t_N=tu/\lambda$).

3 Results and discussion

As our objective is to find the influence of local dispersion on macrodispersion, we use for the longitudinal component the relative difference $\Delta D_{LA} = [D_{LA}(Pe_L,Pe_T,Pe=\infty)/D_{LA}(Pe_L=\infty,Pe_T=\infty,Pe=\infty)] - 1$ between the macrodispersions obtained with local dispersion and with neither dispersion nor diffusion. As the transverse macrodispersion in pure advection cases is null [6], we keep for the transverse component the quantity D_{TA}. Because of its normalization, D_{TA} can be interpreted as the ratio of the transverse macrodispersion to the local transverse dispersion. All values of macrodispersion given hereafter have been checked for convergence on their corresponding time-dependent dispersion chronicle.

3.1 Isotropic local dispersion ($Pe_L=Pe_T$)

ΔD_{LA} and D_{TA} display opposite tendencies. ΔD_{LA} decreases with σ^2 (see Fig.1a) while D_{TA} increases with σ^2 (see Fig. 1b). These tendencies are qualitatively similar to those obtained with semi-analytical approximation methods [16] and to those obtained with diffusion instead of dispersion [6]. For σ^2equal to 0.25 and 1, the semi-analytical approximation and numerical results of the longitudinal macrodispersion are very close together. More precisely the difference is of the order of 4% for $\sigma^2=0.25$ and 8% for $\sigma^2=1$. The close results of the semi-analytical and numerical longitudinal macrodispersions are a partial a posteriori validation of the numerical methodology. For the transverse macrodispersion, values of D_{TA} for $\sigma^2=0.25$ and 1 are at the resolution limit of the numerical methodology and cannot be reliably compared to the analytical approximation. For $\sigma^2=2.25$, the isotropic local dispersion does not induce any discernable effect on the longitudinal macrodispersion. For $\sigma^2\geq4$, the isotropic local dispersion induces a slight reduction of the longitudinal macrodispersion. The reduction is limited to around 30% at most for $\sigma^2=9$ and $Pe_L=Pe_T=10$. The increase of the transverse macrodispersion is much more significant as the transverse macrodispersion is null for pure advection. For σ^2 values larger than 1, the deviation of the semi-analytical and numerical results is larger for the transverse macrodispersion than for the longitudinal macrodispersion. Transverse macrodispersion is specifically triggered by the local dispersion. The macrodispersion is however from 2 to 50 times larger than the local dispersion ($D_{TA}\in[2,50]$). The effect of the local dispersion is amplified by the heterogeneity of permeability as D_{TA} increases with σ^2. D_{TA} also increases with less local dispersion (lower Pe_L values). It does not mean that transverse macrodispersion is lower with more local dispersion but that its amplification is lower with more local dispersion. The amplification is thus linked to the existence of local

dispersion or diffusion rather than to their magnitude. The same trends are observed with diffusion instead of dispersion. As said previously, the effect of isotropic local dispersion is qualitatively similar to the effect of diffusion. For $\sigma^2 \geq 1$, local dispersion like diffusion induces a reduction of the longitudinal macrodispersion and an increase of the transverse macrodispersion.

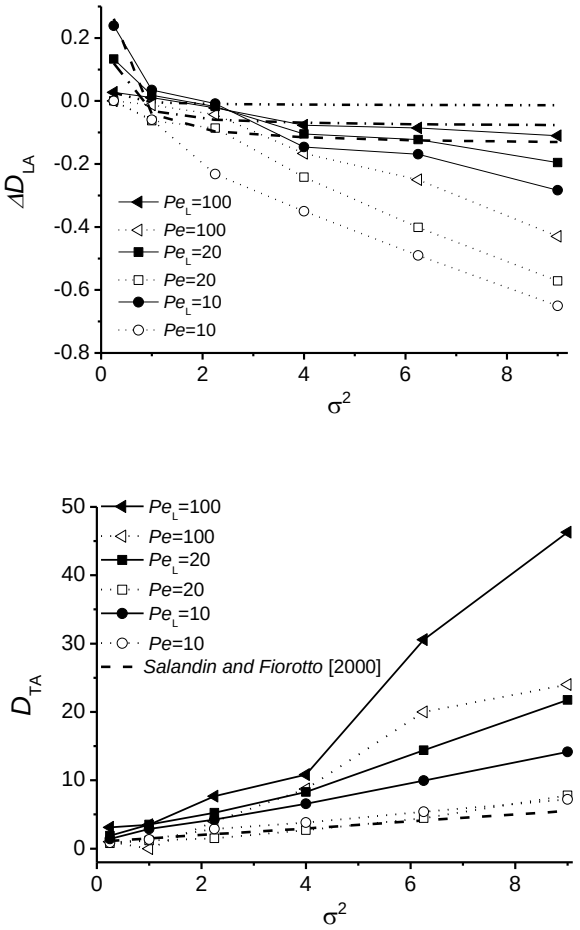

FIG. 1 – (a) Relative difference of longitudinal macrodispersion coefficients and (b) absolute difference of transverse macrodispersion coefficients as functions of σ^2 for various values of *Pe* and $Pe_L=Pe_T$. Dashed lines come from the analytical approximation of *Salandin and Fiorotto* [2000].

We have reported on Fig. 1 the macrodispersions obtained for diffusion with the same Peclet numbers for local dispersion (Pe_L and Pe_T) and for diffusion (*Pe*). The objective is to compare more quantitatively the relative effects of diffusion and dispersion. Globally, diffusion induces a reduction of the longitudinal macrodispersion twice as large as local dispersion. On the contrary the dispersion triggered by permeability heterogeneities amplifies the transverse local dispersion to the transverse macro-dispersion 1.5 to 3 times as much as diffusion. We explain these opposite tendencies 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. The longitudinal macrodispersion is especially sensitive to the solutes trapped in the low velocity zones. Adding diffusion releases them from their trap and significantly reduces the longitudinal macrodispersion [6]. As local dispersion is proportional to velocity, it is less effective than diffusion as a releasing factor and the reduction of the macrodispersion is smaller. In the transverse direction, solutes in the high velocity zones are spread laterally further away with dispersion than with diffusion. This could explain the increase of the transverse macrodispersion.

3.2 Anisotropic pore-scale dispersion ($Pe_L<Pe_T$)

Anisotropic local dispersion has little influence on longitudinal macrodispersion for values of σ^2 smaller or equal to 2.25 (see FIG. 2). For σ^2 equal to 0.25, the modification of dispersion induced by local dispersion is nincreased by 50% when reducing the transverse dispersion by two orders of magnitude, corresponding to less than 10% of the global longitudinal macrodispersion. For σ^2 equal to 1 and 2.25, the longitudinal macrodispersion is close to 0 for isotropic as well as for anisotropic local dispersion. For σ^2 larger than 2.25, anisotropy lets the longitudinal macrodispersion increase (see FIG. 2a). The increase is significant at least for the qualitative influence of dispersion. In fact, for high levels of heterogeneities ies ($\sigma^2>1$), the anisotropic local dispersion ($Pe_L/Pe_T\geq10$) induces an increase of longitudinal macro-dispersion, whereas isotropic local dispersion has the opposite effect, i.e. a decrease of the longitudinal macrodispersion. The same tendencies have been obtained for $Pe_L=10$ and 100. In the transverse direction, a decrease of the transverse local dispersion systematically induces a decrease of the transverse macrodispersion (see FIG. 2b). From the local scale to the macro scale, the reduction decreases with more permeability heterogeneity. For low heterogeneity cases ($\sigma^2\leq1$), the decrease is of the order of 70% for one order of magnitude decrease of the transverse local dispersion (i.e. from $Pe_L/Pe_T=1$ to $Pe_L/Pe_T=10$), the case for which the analytical solution of transport equation predicts a decrease of 67,5%. For the high heterogeneity cases ($\sigma^2>1$), the reduction of the transverse macrodispersion is more limited to at most a factor of 2 for one order of magnitude decrease of the transverse local dispersion.

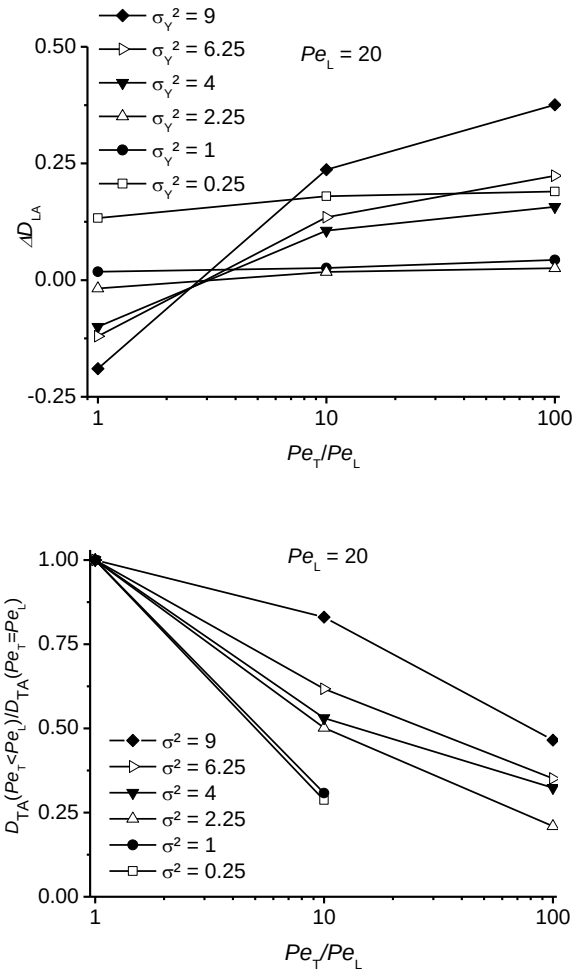

FIG. 2 – (a) ΔD_{LA} and (b) rate between the transverse macrodispersion coefficients obtained with anisotropic local dispersion ($Pe_T>Pe_L$) and without isotropic local dispersion ($Pe_L=Pe_T$) as functions of Pe_L/Pe_T.

4 Conclusion

We find that the contribution of local dispersion to the longitudinal macrodispersion remains highly limited. Quantitatively, the contribution reaches at most 25% for the highest heterogeneity but is more generally

limited to 10%. Qualitatively however, local dispersion may induce opposite effects on the longitudinal macrodispersion. For $\sigma^2>1$, the longitudinal macrodispersion is reduced when the local dispersion is isotropic whereas it increases when the local dispersion is anisotropic, provided that the transverse local dispersion at least one order of magnitude smaller than the longitudinal local dispersion. The transverse macrodispersion only comes from the existence of local dispersion and diffusion. Neglecting the local dispersion would yield a zero transverse macrodispersion. Adding it simply to the estimates without local dispersion leads to strong underestimates of the transverse macrodispersion.The transverse macrodispersion is much larger than the local transverse dispersion. Most of the amplification factors are in the interval [2,15] even if they can reach 50. Surprisingly for $\sigma^2>1$ the decrease of the transverse local dispersion by two orders of magnitude induces only a reduction of the transverse dispersion by at most a factor of 4. It shows the contribution of the longitudinal local dispersion to the transverse macrodispersion.

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