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EVALUATION OF THE DISPERSION PROCESSES IN CONDITIONED TRANSMISSIVITY FIELD

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1 INTRODUCTION

Conditioning on available measures makes the mathematical description of the hydraulic transmissivity field as inhomogeneous even if the original one isn't. Clear examples about multigaussian conditioning[1] shows as, starting from a field that is stationary in the strict sense, the conditioned random function is no more statistically homogeneous being conditioned mean, covariance and variance depending on the spatial position. Obviously velocity fields deduced from the latter are inhomogeneous too[2,3], as shown in papers dealing with nonlocal formalism and non-Darcian flux[4,5].

Among various aspects of conditioning widely discussed in the literature[6,7], we focus the attention on the effects related to the effective dispersion[8] in conditioned log transmissivity fields. This topic has been tackled in the past in a hydraulic transmissivity field of finite correlation length[9] and in self-similar porous formations with a large scale cutoff[10]. While the former describes the impact of an uniform recharge on the conditioning process, in the latter it is shown as a single measurement reduces the difference between ensemble and effective solute moments[8,11], depending the effectiveness in reducing uncertainty on the position of the measurement respect the plume mean trajectory. Respect to these papers, we stress here the role of the flow field inhomogeneity to analyze its impact on the effective dispersion prevision in conditioned transmissivity fields. This goal is reached by use of the stochastic finite element method (SFEM) to handle nonstationarity stemming from the transmissivity conditioning in a finite 2-D domain[12], and by taking into account the mutual relevance of the initial plume finite size and of the inhomogeneity of the flow field in the nonergodic dispersion process[13].

From the analysis of the developed numerical examples, it is shown as the effective dispersion may lead to a reductive forecast of the real plume spreading when, as in conditioned hydraulic transmissivity fields, the spatial stationarity of the flow field is not obeyed.

2 BASIC EQUATIONS

We consider a cloud of inert solute driven by a steady state velocity field $\mathbf{v}(\mathbf{x})$ in a heterogeneous porous medium of constant porosity n. The solute cloud can be viewed as a sum of indivisible particles, each of mass $dM=nC_0(\mathbf{a})d\mathbf{a}$, injected at $t=t_0$ in the volume V_0 being zero the concentration outside, so that the relative concentration in the coordinate $\mathbf{x}$ is defined as $\Delta C=C_0(\mathbf{a})\delta(\mathbf{x}\text{-}\mathbf{X})d\mathbf{a}$, where δ is the Dirac's function. The capital $\mathbf{X}=\mathbf{X}(t;\mathbf{a},t_0)$ is the particle trajectory originating from $\mathbf{X}=\mathbf{a}$ at $t=t_0$ and it can be computed as

$$\mathbf{X}(t;\mathbf{a},t_0)=\mathbf{a}+\int_{t_0}^{t}\mathbf{v}\left[\mathbf{X}(t';\mathbf{a},t_0)\right]dt \tag{1}$$

The relationship (1) is written under the hypothesis that the dispersion phenomenon is dominated by the velocity field spatial variability, that is neglecting the pore scale effects, and according to the linear analysis the $\mathbf{X}_0$ zero-th and the $\mathbf{X}'$ first-order terms can be obtained from

$$\begin{aligned}&dX_{0i}/dt=v_{0i}(\mathbf{X}_0)\\&dX_i'/dt=v_i(\mathbf{X}_0)+(X_j\nabla)v_{0i}(\mathbf{X}_0),\qquad i,j=1,2,3\end{aligned} \tag{2}$$

In a statistically homogeneous flow field the zero-th order term is constant and its derivative becomes zero, while in the general case the solution of (2) is given by[14]

$$X_i'(t)=\Phi_{ik}(t,t_0)X_i'(t_0)+\int_{t_0}^{t}\Phi_{ik}(t,t')v_i'(\mathbf{X}_0)dt',\qquad i,k=1,2,3 \tag{3}$$

where $\mathbf{\Phi}$ is the state transition matrix satisfying the homogeneous equation $d\mathbf{\Phi}/dt=\mathbf{B}(t)\mathbf{\Phi}(t,t_0)$ with initial condition $\mathbf{\Phi}(t_0,t_0)$ given by the identity matrix. The element $B_{ij}(t)$ of $\mathbf{B}$ is the derivative of the zero-th order Lagrangian velocity in the i-th direction with respect to the trajectory $X_j(t)$, evaluated at the instantaneous particle mean position

$$B_{ij}(t)=\left.\frac{\partial v_{0i}\left[\mathbf{X}(t)\right]}{\partial X_j(t)}\right|_{\mathbf{X}(t)=\mathbf{X}_0(t)},\qquad i,j=1,2,3 \tag{4}$$

If the displacement perturbation at the initial state is $\mathbf{X}'(t_0)=0$, for instance at the time of a known release ($t_0=0$), one can write the second moment of two particles displacement as

$$\begin{aligned}X_{ij}(t;\mathbf{a},\mathbf{b},t_0)&=\langle X_i'(t;\mathbf{a},t_0)X_j'(t;\mathbf{b},t_0)\rangle\\&=\langle\int_{t_0}^{t}\Phi_{ik}(t,t')v_k'\left[\mathbf{X}_0(t';\mathbf{a},t_0)\right]dt'\int_{t_0}^{t}\Phi_{jm}(t,t'')v_m'\left[\mathbf{X}_0(t'';\mathbf{b},t_0)\right]dt''\rangle\\&=\int_{t_0}^{t}dt'\int_{t_0}^{t}dt''\,\Phi_{ik}(t,t')\Phi_{jm}(t,t'')C_{v_{km}}(t',t'';\mathbf{a},\mathbf{b},t_0),\qquad i,j,k,m=1,2,3\end{aligned} \tag{5}$$

where, according to the fist-order analysis, $C_{vkm}(t',t'';\mathbf{a},\mathbf{b},t_0)$ is the Eulerian velocity covariance evaluated at the coordinates $\mathbf{x}_1=\mathbf{X}_0(t';\mathbf{a},t_0)$ and $\mathbf{x}_2=\mathbf{X}_0(t'';\mathbf{b},t_0)$.

In the case of stationary and unidirectional flow field, $\mathbf{B}(t)=\mathbf{0}$, $\mathbf{\Phi}(t_0,t_0)$ reduces to the identity matrix and the computation of (5) becomes straightforward[12].

Anyway, as previously stated, our interest is here devoted to the expected value of the second-order spatial moment tensor S_{ij} that is related to the effective dispersion. In the literature[8,11] the effective (or actual) dispersion, is compared with the ensemble one that follows from the second moment of the ensemble-averaged concentration distribution given by (5). Defined as $\tilde{X}_i = X_i - a_i$ the particle's displacement relative to the initial position, the expected value of the second-order spatial moment tensor S_{ij} can be written as[13]

$$\begin{aligned}\langle S_{ij}\left[t;V_0(\mathbf{x}),t_0\right]\rangle = \frac{1}{V_0}\int_{V_0}\langle X_i' X_j'\rangle d\mathbf{a} - \langle R_i' R_j'\rangle \\ +\left[\frac{1}{V_0}\int_{V_0}\langle a_i a_j\rangle d\mathbf{a} - \bar{a}_i\bar{a}_j\right] \\ +\left[\frac{2}{V_0}\int_{V_0} a_i\langle\tilde{X}_j\rangle d\mathbf{a} - \frac{2\bar{a}_i}{V_0}\int_{V_0}\langle\tilde{X}_j\rangle d\mathbf{a}\right] \\ +\left[\frac{1}{V_0}\int_{V_0}\langle\tilde{X}_i\rangle\langle\tilde{X}_j\rangle d\mathbf{a} - \frac{1}{V_0}\int_{V_0}\langle\tilde{X}_i\rangle d\mathbf{a}\frac{1}{V_0}\int_{V_0}\langle\tilde{X}_j\rangle d\mathbf{a}\right], \quad i,j=1,2,3\end{aligned} \tag{6}$$

where the superscript refers to the center of mass $\bar{\mathbf{a}}$ of the initial solute volume V_0, while R'_i describes the space evolution of the same center of mass for $t>t_0$. For brevity in the following the three terms in square brackets of (6) are referred as $S_{ij}(0)$, M_{ij} and Q_{ij} respectively. $S_{ij}(0)$ is the inertia moment of the plume starting position, while M_{ij} and Q_{ij} derive from the lack of flow field stationarity. More in depth M_{ij} is a memory term related to the initial state of the solute plume, while Q_{ij} is related to the fluctuations of the velocity ensemble average that may become relevant in conditioned log transmissivity fields.

To obtain a more in depth understanding, from the results of the numerical simulations here developed, the role of the terms related to the flow field statistical inhomogeneity M_{ij} and Q_{ij} in a conditioning procedure will be made explicit.

3 NUMERICAL EXAMPLES AND SPATIAL MOMENT RESULTS

3.1 Synthetic reference aquifer and conditional simulations

We develop the conditioning on a hydraulic log transmissivity field $Y=\ln T$ with isotropic exponential function $C_Y(|\mathbf{a}-\mathbf{b}|)=\sigma_Y^2\exp[-(|\mathbf{a}-\mathbf{b}|)/\lambda]$, being σ_Y^2 the variance, λ the correlation length and $|\mathbf{a}-\mathbf{b}|$ the lag distance between two points. The domain is a square plane of lateral size $L=20\lambda$ discretized into 80×80 elements, with the following boundary conditions: piezometric head $H=100\lambda$ on the left side ($x_1=0$) and $H=98\lambda$ on the right side ($x_1=20\lambda$), no flux in the other two sides ($x_2=0$ and $x_2=20\lambda$). The solute source is a line normal to the mean flow direction centered at the point $x_1=0.125\lambda$, $x_2=9.875\lambda$, and four different lengths $\ell=1$, 3, 6 and 9λ are taken into account in the experiments.

A synthetic reference aquifer was simulated by ascribing at each square element of the computational grid the log transmissivity value obtained from one single unconditional realization, generated by setting $\langle Y \rangle = \ln(10)$ and $\sigma_Y^2 = 0.2$. Because of the finite size of the domain, the ergodic condition was only approximately met and the spatial statistics return a log transmissivity mean and variance equal to 2.26 and 0.202 respectively. Conditioned log transmissivity fields were generated by the sequential Gaussian simulator SGSIM[15] on the Y values extracted from the synthetic aquifer at evenly spaced points. Three different lags between measurement points $d=6\lambda$, $d=4\lambda$ and $d=2\lambda$ are considered giving 16, 25 and 100 conditioning data respectively on the total number of 6400 log transmissivity values. To ensure the accuracy in the reproduction of the log transmissivity statistical moments the number of realizations was set equal to 2000. For the purpose of comparison the unconditional case where the flow nonstationarity derives only from the boundary influence was considered also.

3.2 Time evolution of solute spatial moments

The numerical solution of the flow problem is achieved by the SFEM approach[12] on the basis of the previously computed statistical moments of conditioned log transmissivity fields. This let us able to evaluate by integration the second moment of two particles displacement (5) and each term of (6).

The evolution of the plume centroid expected values is reported in Figure 1 and compared with the path obtained in the synthetic reference aquifer. The centroid trajectory deviates from the unconditional behavior, a straight line characterized by constant velocity, and as the number of conditioning points increases approaches the actual path. Moreover from the comparison between Figure 1 a) and b) one can note that as the plume initial size increases differences between actual path and other trajectory expected values reduce.

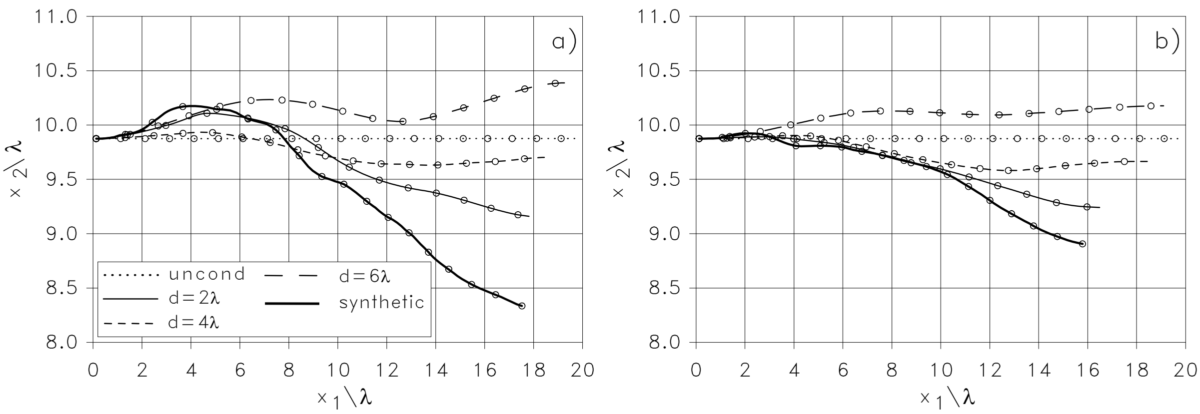

Figure 1: Trajectory expected values of the plume centroid for different d values and solute source sizes: a) $\ell = 1\lambda$ and b) $\ell = 9\lambda$. Circles represent the centroid positions at unitary dimensionless travel time steps.

This is mainly due to the modification of the actual path moving from $\ell = 1$ to 9λ, while only the case with $d=2\lambda$ seems to be significantly affected by the increase of the conditioning point number. From the result one can argue that: *i*) the prediction of the solute path originating from a small injection volume requires a large number of conditioning data; *ii*) in this case only early travel time behavior can be forecasted, and *iii*) it is easier to assess the mean path of a large solute injection, since a satisfactory approximation can be obtained with a less dense grid of conditioning data, while the late travel time is always difficult to be properly reproduced. All these results were to be expected, anyway they are relevant for practical purposes when it is required to predict by conditioning the mean spatial evolution of a pollutant source of finite dimension, and to have an idea about the convergence to the synthetic path, shadowed by the longitudinal mean velocity fluctuations, as a function of conditioning point spatial density.

Figure 2 illustrates the spatial moments referred as $\langle S_{11}\rangle - S_{11}(0)$, $M_{11}+Q_{11}$ and R_{11} for the case $\ell = 9\lambda$ and different d values, as a function of the dimensionless travel time $t' = t\langle v_1\rangle/\lambda$, where $\langle v_1\rangle$ is the unconditional mean velocity parallel to x_1. The unconditional solution and the spatial second moment computed for the synthetic case are shown for comparison.

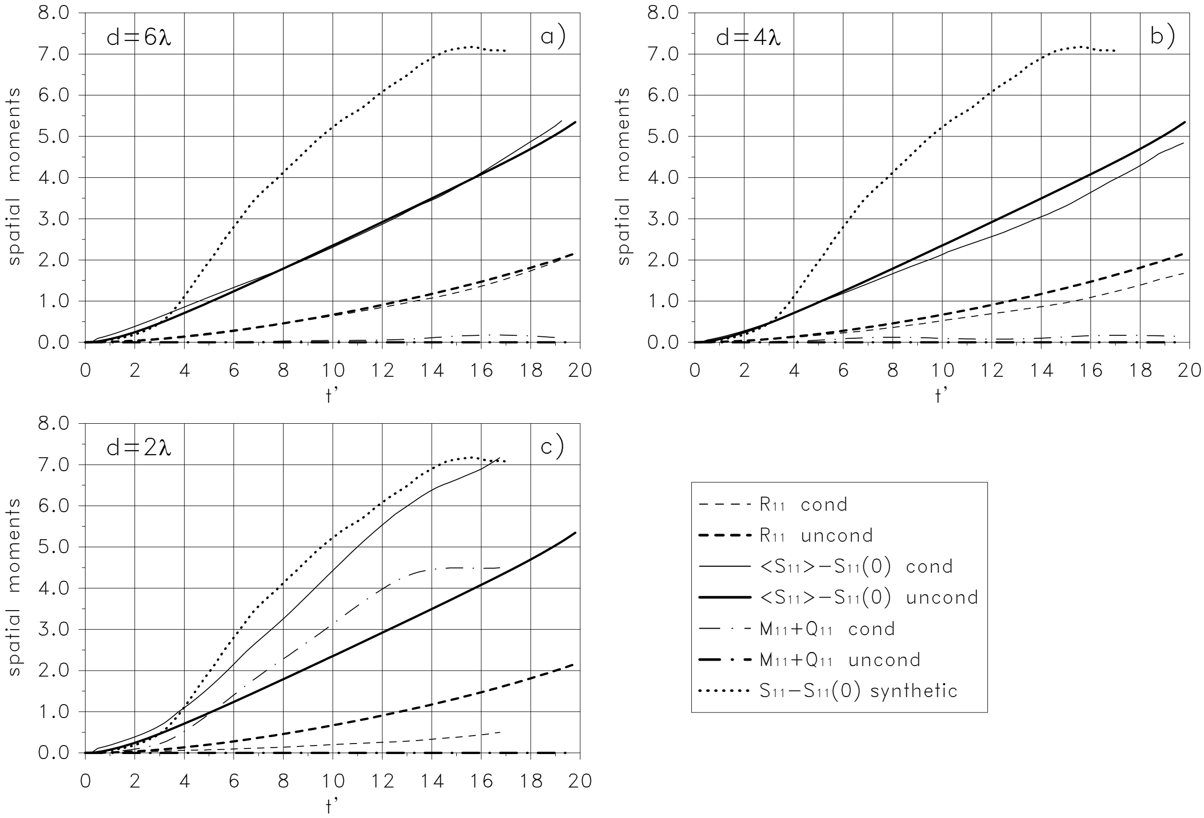

Figure 2: Longitudinal second spatial moments R_{11}, $M_{11}+Q_{11}$ and $\langle S_{11}\rangle - S_{11}(0)$ as a function of travel time for initial solute source size $\ell = 9\lambda$: a) d=6λ, b) d=4λ and c) d=2λ

As expected, increasing the number of conditioning points the uncertainty in the centroid trajectory reduces and R_{11} in the conditional case becomes smaller than the corresponding unconditional result. The moments M_{11} and Q_{11} related to the Lagrangian flow field spatial stationarity are zero in the unconditional case being constant the expected value of the velocity field. Under conditioning the expected value of conditional velocity is not spatially constant, the mean particle trajectories deviate from the straight line and the term Q_{11} becomes positive. In our experiments M_{11} remains always zero, being the source aligned along the x_2 axis. In the case d=6λ the conditioning influence on the spatial moments is quite limited and differences between conditional and unconditional results are negligible. For d=4λ the increase of Q_{11} is still slight and the second moment $\langle S_{11}\rangle$ is smaller than the unconditional case. Instead for d=2λ also if R_{11} reduces, the large increase of Q_{11} leads to values of $\langle S_{11}\rangle$ larger than the unconditional case and close to the synthetic one.

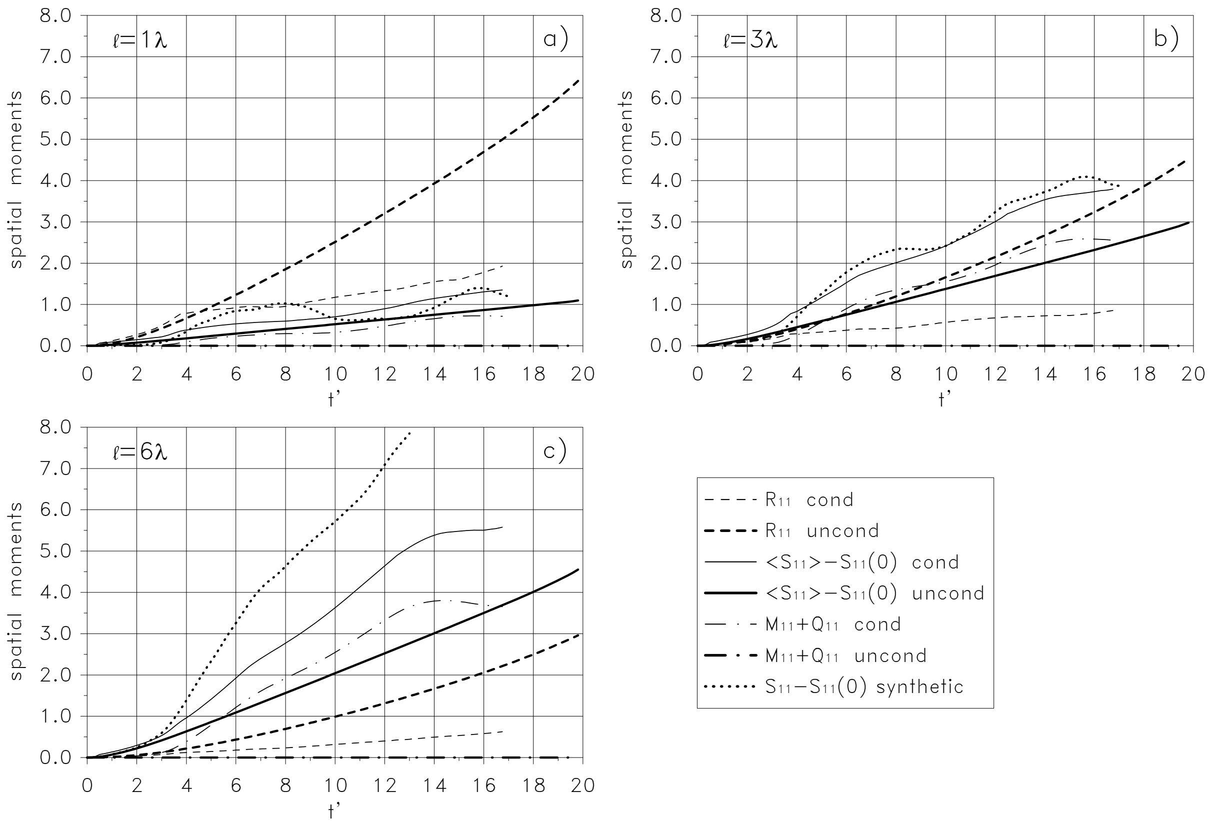

Figure 3: Longitudinal second spatial moments R_{11}, M_{11}+Q_{11} and $\langle S_{11}\rangle - S_{11}(0)$ as a function of travel time for d=2λ and different initial solute source sizes: a) ℓ = 1λ, b) ℓ = 3λ and c) ℓ = 6λ

Note that to capture the behavior of the synthetic actual dispersion a dense grid of conditioning points is required, resulting substantially unaffected the conditional $\langle S_{11}\rangle$ behavior in the cases d=6λ and d=4λ. To reach a good estimate the R_{11} decrease is irrelevant, and only the growth of Q_{11} for d=2λ leads to a proper approximation of the wished goal.

The solute spatial moments obtained for d=2λ and ℓ=1, 3, and 6λ are reported in Figure 3 in comparison with the unconditional solution. The smaller size of the initial solute length enhances the different contributes related to the statistical inhomogeneity of the flow field and the lack of ergodicity in the transport. In absence of conditioning the uncertainty in the centroid trajectory R_{11} reduces, while the moments $\langle S_{11} \rangle$ increases with the source length, being M_{11} and Q_{11} equal to zero. Conditioning with d=2λ causes a general decrease of the centroid uncertainty R_{11}, while the Q_{11} enhancement dominates the growth of the effective spreading. From (6) it is easy to recognize that the relevance of Q_{11} is strictly related to both the initial solute size ℓ and the spacing d between conditioning points. As the ratio d/ℓ increases the expected values of particle trajectories become unaffected by the spatial integration and Q_{11} vanishes. To move from the ensemble to the effective dispersion the primary role is played by the uncertainty of center of solute mass R_{11}, while the Q_{11} term, related to the lack of statistical homogeneity of the velocity field, has a dominant part to approach the synthetic dispersion starting from the effective one. Anyway, the finite size of the initial solute body and the number of conditioning points, that lead to nonergodic and inhomogeneous conditions, have a combined effect related to the ratio d/ℓ that may significantly affect the transport process.

4 CONCLUSIONS

Under conditioning the centroid trajectory expected value deviates from the unconditional behavior and approaches the actual path as the number of conditioning points increases. The uncertainty in the centroid trajectory reduces becoming smaller than the corresponding unconditional result. Since the mean particle trajectories deviate from the straight line, the transport moments related to the lack of spatial stationarity of the flow field become significant. This fact leads to a solute dispersion larger than the unconditional case and closer to the synthetic one. In other words, in velocity fields that doesn't obey the statistical homogeneity, the effective dispersion, evaluated as the difference between ensemble mean and trajectory uncertainty may lead to a reductive forecast of the real plume spreading.

The proper reproduction of the actual path is significantly affected by the number of conditioning points and the prediction of the solute path originating from a small injection volume requires a large number of data. In this case only early travel time behavior can be forecasted, while it is easier to assess the mean path of a large solute injection. Anyway the late travel time is always difficult to be properly reproduced.

The dispersion process is affected by the ratio between the spacing between conditioning points and the initial solute size d/ℓ that straight affects the M_{ij}+Q_{ij} term related to the flow statistical inhomogeneity. As this ratio increases the expected values of particle trajectories result substantially unaffected by the spatial integration and the M_{ij}+Q_{ij} vanishes. To move from the ensemble to the effective dispersion the primary role is played by the uncertainty of center of solute mass R_{ij}, while the M_{ij}+Q_{ij} term has a dominant part to approach the synthetic dispersion starting from the effective one. This result with that one related to the solute mean path is relevant for all practical purposes when it is required to predict by conditioning the mean spatial evolution and the dispersion of a pollutant source of finite initial size.

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