Erratum: Effective dispersion in temporally fluctuating flow through a heterogeneous medium [Phys. Rev. E 68, 036310 (2003)]

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In our paper we studied transport of a passive solute in the flow through a heterogeneous medium under temporal fluctuations of the flow boundary conditions. We employed a stochastic modeling approach for both the spatial medium heterogeneities and the temporal flow fluctuations. Using perturbation theory in the spatiotemporal fluctuations of the flow velocity, we derived explicit expressions for the effective dispersion coefficients. We concluded that temporal fluctuations in direction of the mean flow enhance solute dispersion both in longitudinal and transverse direction.

Recently, we have conducted numerical simulations [1] of transport in temporally fluctuating flow through heterogeneous porous media. Contrary to our paper, we have found that temporal fluctuations in longitudinal direction have only a subleading effect on both longitudinal and transverse dispersion. Therefore, we have revised our previous derivation. We found that the discrepancy between the analytical results and the numerical observations can be traced back to the disregard of certain contributions in the perturbation expansion for the dispersion coefficients.

These terms are caused by the specific form of the flow field $\mathbf{u}(\mathbf{x},t)$ through a heterogeneous medium. The field $\mathbf{u}(\mathbf{x},t)$ can be decomposed into a term that fluctuates in time only, and one that fluctuates in space and time (e.g., [2] and this paper),

$$\mathbf{u}(\mathbf{x},t) = \mathbf{u}(t) - \mathbf{u}'(\mathbf{x},t). \tag{1}$$

The space-ensemble average, denoted here by an overbar, of the fluctuation $\overline{\mathbf{u}'(\mathbf{x},t)} = \mathbf{0}$ is zero. In our paper, we identified the terms arising from the spatiotemporal fluctuations $\mathbf{u}'(\mathbf{x},t)$ as macroscopic contributions to both the longitudinal and transverse dispersion coefficients. However, as outlined in the following, for longitudinal fluctuations $[u_i(t) = \delta_{i1}u(t)]$ cross contributions between $\mathbf{u}(t)$ and $\mathbf{u}'(\mathbf{x},t)$ cancel with these terms. Thus, we find that there is actually no sizable contribution to the dispersion coefficients for temporal flow fluctuations in the direction of the mean flow.

Nevertheless, the results of our paper are valid for dispersion in a spatiotemporal random flow field of the structure,

$$\mathbf{u}(\mathbf{x},t) = \mathbf{u} - \mathbf{u}'(\mathbf{x},t), \tag{2}$$

that is, for a flow field that can be decomposed into the constant average and fluctuations in space and time with $\overline{\mathbf{u}'(\mathbf{x},t)} = \mathbf{0}$. Dispersion in such random velocity fields finds applications in, for example, plasma turbulence, oceanography, and atmospheric transport [3–6].

In the following, we present the derivation of the expressions for the dispersion coefficients including the terms omitted in our original paper. We compare the analytical expressions to numerical random walk particle tracking simulations of transport in random velocity fields of type (1) and (2).

The starting point is the Fokker-Planck equation for the concentration $c(\mathbf{x},t)$,

$$\frac{\partial c(\mathbf{x},t)}{\partial t} + \mathbf{u}(\mathbf{x},t)\cdot\nabla c(\mathbf{x},t) - D\nabla^2 c(\mathbf{x},t) = 0. \tag{3}$$

The dispersion coefficient D is constant. As boundary conditions we assume vanishing $c(\mathbf{x},t)$ at infinity. The initial condition is $c(\mathbf{x},t=0) = \delta(\mathbf{x})$.

The incompressible random flow field $\mathbf{u}(\mathbf{x},t)$ through a heterogeneous porous medium is given by the Darcy equation $\mathbf{u}(\mathbf{x},t) = -K(\mathbf{x})\nabla h(\mathbf{x})$, in which $K(\mathbf{x})$ is hydraulic conductivity and $h(\mathbf{x})$ hydraulic head. The log-hydraulic conductivity $f(\mathbf{x}) = \ln[K(\mathbf{x})]$ is modeled as a stationary Gaussian random field. The flow field $\mathbf{u}(\mathbf{x},t)$ is approximated by the linearized solution of the Darcy equation (e.g., this paper). It can be decomposed into

$$u_i(\mathbf{x},t) = u\delta_{i1} - u\nu_i(t) - u_i'(\mathbf{x},t). \tag{4}$$

The spatiotemporal fluctuations $u_i'(\mathbf{x},t)$ can be further decomposed into a term that fluctuates in space only and one that fluctuates in space and time,

$$u_i'(\mathbf{x},t) = u_{i1}'(\mathbf{x}) - u_{il}'(\mathbf{x})\nu_l(t). \tag{5}$$

We define the $u_{il}'(\mathbf{x})$ through their Fourier transforms as $\tilde{u}_{il}'(\mathbf{k}) = up_{il}(\mathbf{k})\tilde{f}'(\mathbf{k})$ with $p_{il}(\mathbf{k}) \equiv \delta_{il} - k_i k_l/k^2$. We sum over repeated indices. For the definition of the Fourier transform, see the original paper.

The stationary random field $\boldsymbol{\nu}(t)$ quantifies the normalized fluctuations of the spatial mean hydraulic gradient. Its time average is zero by definition $\langle\boldsymbol{\nu}(t)\rangle = 0$. The ensemble average over the temporal random process is denoted by the angular brackets; the average over all realizations of the random medium is denoted by the overbar.

The correlation functions are $\langle\nu_l(t)\,\nu_m(t')\rangle = \sigma_{\nu\nu}^2 C_{lm}^{\nu\nu}(t-t')$ and $\overline{f'(\mathbf{x})\,f'(\mathbf{x}')} = \sigma_{\rm ff}^2 C^{\rm ff}(\mathbf{x}-\mathbf{x}')$, with $\sigma_{\nu\nu}^2$ and $\sigma_{\rm ff}^2$ the respective variances. They are characterized by the correlation time τ and the correlation length l, respectively. The (spatial) correlation of the velocity fluctuations in Fourier space can be

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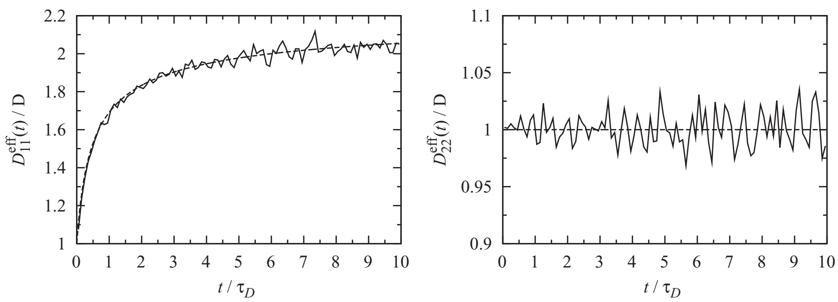

FIG. 1. Longitudinal and transverse effective dispersion coefficients for $d = 2$ dimensions in the velocity field (4) obtained from (solid) numerical random walk particle tracking simulations for $\sigma_{\rm ff}^2 = 10^{-2}$ and $\sigma_{\nu\nu}^2 = 10^{-1}$ and (dashed) the perturbation theory expression (30) for $D_{11}^{\rm eff}(t)$. The transverse coefficient is essentially given by the local dispersion coefficient.

written as $\overline{\widetilde{u}'_i(\mathbf{k},t)\widetilde{u}'_j(\mathbf{k}',t)} = \sigma_{\rm ff}^2 \widetilde{C}^{\rm uu}_{ij}(\mathbf{k},t,t')\widetilde{C}^{\rm ff}(\mathbf{k})(2\pi)^d\delta(\mathbf{k}+\mathbf{k}')$, where we defined

$$\widetilde{C}^{\rm uu}_{ij}(\mathbf{k},t,t') = [\widetilde{C}_{i1j1}(\mathbf{k}) + \widetilde{C}_{iljm}(\mathbf{k})\nu_l(t)\nu_m(t') - \widetilde{C}_{i1jm}(\mathbf{k})\nu_m(t') - \widetilde{C}_{ilj1}(\mathbf{k})\nu_l(t)], \quad (6)$$

with $\widetilde{C}_{iljm}(\mathbf{k}) = u^2 p_{il}(\mathbf{k}) p_{jm}(\mathbf{k})$.

Characteristic time scales are the correlation time τ of the fluctuations of $\nu(t)$, the advection scale $\tau_u = l/u$, and the dispersion scale $\tau_D = l^2/D$. The ratio between advection scale and dispersion scales defines the inverse Péclet number $\epsilon = \tau_u/\tau_D$. The Kubo number $\kappa = \tau/\tau_u$ compares correlation and advection scales.

Solute dispersion is measured by the effective dispersion coefficients (e.g., this paper),

$$D_{ij}^{\rm eff}(t) = -\frac{1}{2}\frac{d}{dt}\frac{\partial^2}{\partial k_i \partial k_j}\overline{\langle \ln[\widetilde{c}(\mathbf{k},t)]\rangle}|_{\mathbf{k}=\mathbf{0}}, \quad (7)$$

and the ensemble dispersion coefficients (e.g., this paper),

$$D_{ij}^{\rm ens}(t) = -\frac{1}{2}\frac{d}{dt}\frac{\partial^2}{\partial k_i \partial k_j}\langle \ln[\overline{\widetilde{c}(\mathbf{k},t)}]\rangle|_{\mathbf{k}=\mathbf{0}}. \quad (8)$$

The difference between the two quantities measures the evolution of the sample-to-sample fluctuations of the center-of-mass position, $D_{ij}^{\rm cm}(t) = D_{ij}^{\rm ens}(t) - D_{ij}^{\rm eff}(t)$.

Using the decomposition (4) of $\mathbf{u}(\mathbf{x},t)$ in (3) and performing the Fourier transform we derive the equivalent integral equation,

$$\widetilde{c}(\mathbf{k},t) = \widetilde{c}_0(\mathbf{k},t|0) - \int_{k'}\int_0^t dt'\widetilde{c}_0(\mathbf{k},t|t') i\mathbf{k}\cdot\widetilde{\mathbf{u}}'(\mathbf{k}',t')\widetilde{c}(\mathbf{k}-\mathbf{k}',t'). \quad (9)$$

We use the short-hand notation $\int_k = \int d^dk/(2\pi)^d$ with d the dimensionality of space. The propagator $\widetilde{c}_0(\mathbf{k},t|t')$ is given by

$$\widetilde{c}_0(\mathbf{k},t|t') = \widetilde{g}_0(\mathbf{k},t-t')\exp\left[-iu\mathbf{k}\cdot\int_{t'}^t dy\boldsymbol{\nu}(y)\right], \quad (10)$$

with $\widetilde{g}_0(\mathbf{k},t) = \exp(-Dk^2t + {\rm i}k_1ut)$ the propagator of the homogeneous transport equation, that is, for $u_i(\mathbf{x},t) = u\delta_{i1}$ in (3). Iteration of (9) gives a perturbation series in $\widetilde{\mathbf{u}}'(\mathbf{k},t)$.

We insert the expansion of (9) in (7) and (8) and expand the logarithms up to second order in $\widetilde{\mathbf{u}}'(\mathbf{k},t)$. The resulting expressions then are averaged and only contributions up to order $\sigma_{\rm ff}^2\sigma_{\nu\nu}^2$ are retained. Thus, we obtain

$$D_{ij}^{\rm ens}(t) = D_{ij} + \sigma_{\rm ff}^2\int_{k'}\widetilde{C}^{\rm ff}(\mathbf{k}')\mathcal{F}_{ij}^{+}(\mathbf{k}',t), \quad (11)$$

$$D_{ij}^{\rm cm}(t) = \sigma_{\rm ff}^2\int_{k'}\exp(-2\mathbf{k}'\mathbf{D}\mathbf{k}'t)\widetilde{C}^{\rm ff}(\mathbf{k}')\mathcal{F}_{ij}^{-}(\mathbf{k}',t), \quad (12)$$

where we defined the auxiliary functions,

$$\mathcal{F}_{ij}^{\pm}(\mathbf{k}',t) = I_{ij}^{(1)}(\mathbf{k}',t) + \sigma_{\nu\nu}^2\sum_{l,m=1}^{d}\left[I_{ijlm}^{(2)}(\mathbf{k},t) - I_{ijlm}^{(3)}(\mathbf{k}',t) - 2I_{ijlm}^{(4)}(\mathbf{k},t)\right], \quad (13)$$

together with

$$I_{ij}^{(1)}(\mathbf{k}',t) = \int_0^t dt'\widetilde{C}_{i1j1}(\mathbf{k}')\widetilde{g}_0(\mp\mathbf{k}',\pm t'), \quad (14)$$

$$I_{ijlm}^{(2)}(\mathbf{k}',t) = \int_0^t dt'\widetilde{C}_{iljm}(\mathbf{k}')C_{lm}^{\nu\nu}(t')\widetilde{g}_0(\mp\mathbf{k}',\pm t'), \quad (15)$$

$$I_{ijlm}^{(3)}(\mathbf{k}',t) = \int_0^t dt'\widetilde{C}_{i1j1}(\mathbf{k}')\widetilde{g}_0(\mp\mathbf{k}',\pm t')u^2k'_lF_{lm}(t')k'_m, \quad (16)$$

$$I_{ijlm}^{(4)}(\mathbf{k}',t) = \int_0^t dt'\widetilde{C}_{i1jm}(\mathbf{k}')\widetilde{g}_0(\mp\mathbf{k}',\pm t')\times iuk'_lG_{lm}(t'). \quad (17)$$

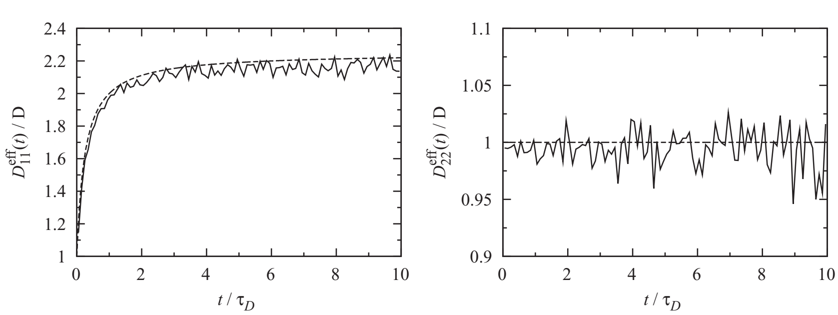

FIG. 2. Longitudinal and transverse effective dispersion coefficients for $d = 3$ in the velocity field (4). The setup is the same as for Fig. 1.

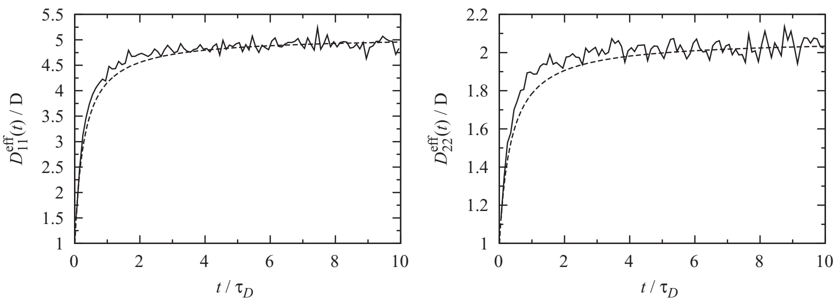

FIG. 3. Longitudinal and transverse effective dispersion coefficients for $d = 2$ dimensions in the velocity field (34) obtained from (solid) numerical random walk particle tracking simulations for $\sigma_{\rm ff}^2 = 10^{-1}$ and $\sigma_{vv}^2 = 1$ and (dashed) the corresponding perturbation theory expressions from our paper.

We furthermore defined

$$F_{lm}(t') = \int_0^{t'} dy \int_0^{y} dy' C_{lm}^{vv}(y'), \tag{18}$$

$$G_{lm}(t') = \int_0^{t'} dy C_{lm}^{vv}(y). \tag{19}$$

Note that the contributions due to (16) and (17) were not taken into account in our paper. These contributions originate from the expansion of the exponential on the right side of (10). For a velocity field of type (2) this term is not present and the only contributions to the dispersion coefficients are given by (14) and (15).

For fluctuations in one direction only, (13) reads as

$$\mathcal{F}_{ij}^{\pm}(\mathbf{k}',t) = I_{ij}^{(1)}(\mathbf{k}',t) + \sigma_{vv}^2 \big[I_{ij11}^{(2)}(\mathbf{k}',t) - I_{ij11}^{(3)}(\mathbf{k}',t) - 2 I_{ij11}^{(4)}(\mathbf{k}',t) \big]. \tag{20}$$

Expanding the contributions $I_{ij11}^{(3)}(\mathbf{k},t)$ and $I_{ij11}^{(4)}(\mathbf{k},t)$ by integration by parts, we derive

$$\mathcal{F}_{ij}^{\pm}(\mathbf{k}',t) = \int_0^t dt' \widetilde{C}_{i1j1}(\mathbf{k}') \widetilde{g}_0(\mp\mathbf{k}',\pm t') - \sigma_{vv}^2 \sum_{n=1}^{4} A_n^{\pm}(\mathbf{k}',t), \tag{21}$$

where the first contribution on the right side is identical to the one for steady flow (e.g., [7]). The remaining contributions are given by

$$A_1^{\pm}(\mathbf{k}',t) = -\widetilde{C}_{i1j1}(\mathbf{k}') \widetilde{g}_0(\mp\mathbf{k}',\pm t) \frac{u^2 {k_1'}^2}{\pm \mathbf{k}'\mathbf{D}\mathbf{k}' + iuk_1'} F_{11}(t), \tag{22}$$

$$A_2^{\pm}(\mathbf{k}',t) = \int_0^t dt' \widetilde{C}_{i1j1}(\mathbf{k}') \widetilde{g}_0(\mp\mathbf{k}',\pm t') \times \frac{\pm iuk_1' D k'^2}{\pm D k'^2 + iuk_1'} G_{11}(t'), \tag{23}$$

$$A_3^{\pm}(\mathbf{k}',t) = -\widetilde{C}_{i1j1}(\mathbf{k}') \widetilde{g}_0(\mp\mathbf{k}',\pm t) \frac{iuk_1'}{\pm D k'^2 + iuk_1'} F_{11}(t), \tag{24}$$

$$A_4^{\pm}(\mathbf{k}',t) = -\int_0^t dt' \widetilde{C}_{i1j1}(\mathbf{k}') \widetilde{g}_0(\mp\mathbf{k}',\pm t') \times \frac{\pm D k'^2}{\pm D k'^2 + iuk_1'} C_{11}^{vv}(t'). \tag{25}$$

We consider now the leading-order behavior for small inverse Péclet number $\epsilon \ll 1$ and times large compared to the advection scale, $t \gg \tau_u$. The contributions due to (23) and (25) are of the order of the inverse Péclet number and thus subleading. The contributions to the dispersion coefficients due to (22) and (24) are given by

$$\delta^{(l)} D_{ij}^{\pm} = \sigma_{\rm ff}^2 \sigma_{vv}^2 \int_{k'} \widetilde{C}^{\rm ff}(\mathbf{k}') A_l^{\pm}(\mathbf{k}',t) \tag{26}$$

for $l = 1,3$. In order to evaluate these contributions, we specify the Gaussian correlation functions $\widetilde{C}^{\rm ff}(\mathbf{k}) = (2\pi)^d \exp(-k^2 l^2/2)$ and $C_{11}^{vv}(t) = \exp[-t^2/(2\tau^2)]$.

In the limit $\epsilon \ll 1$, we obtain for $\delta^{(1)} D_{ij}^{\pm}(t)$,

$$\delta^{(1)} D_{ij}^{\pm}(t) = -\sigma_{\rm ff}^2 \sigma_{vv}^2 F_{11}(t) (2\pi)^{d/2} l^d \int_{k'} \exp(-ik_1' l t/\tau_u) \times \exp(-k'^2 a^{\pm} l^2/2) iuk_1' \widetilde{C}_{i1j1}(\mathbf{k}') + \cdots, \tag{27}$$

where the dots denote subleading contributions of order ϵ. Note that $a_n^+ = 1$ and $a_n^- = 1 + 4t/\tau_D$. We rescale $k_i = k_i' l_1(t/\tau_u)$ and take the limit $t/\tau_u \to \infty$ under the integral. This gives

$$\delta^{(1)} D_{ij}^{\pm}(t) = -F_{11}(t)(t/\tau_u)^{-d-1} \sigma_{\rm ff}^2 \sigma_{vv}^2 (2\pi)^{d/2} l^{-1} \times \int_k iuk_1 \widetilde{C}_{i1j1}(\mathbf{k}) \exp(-ik_1) + \cdots. \tag{28}$$

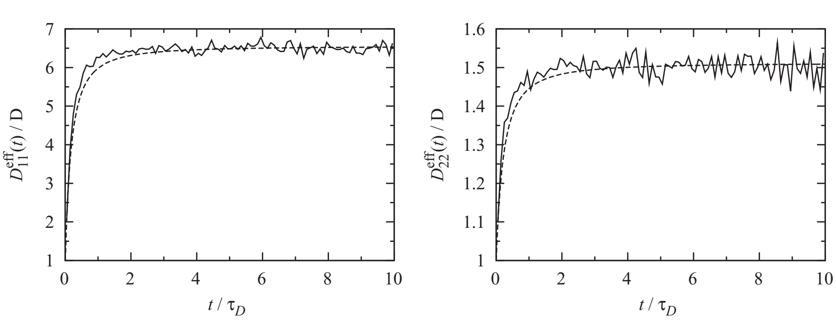

FIG. 4. Longitudinal and transverse effective dispersion coefficients for $d = 3$ dimensions in the velocity field (34). The setup is the same as for Fig. 3.

The remaining integral is finite. Furthermore, as $F_{11}(t)$ scales as $t\tau$ at times $t \gg \tau$, we obtain that $\delta^{(1)} D_{ij}^{\pm}(t)$ scales as $(t/\tau_u)^{-d}$. Thus, it is subleading for $t \gg \tau_u$.

For the contribution $\delta_A^{(3)} D_{ij}^{\pm}(t)$, the reasoning is similar. We obtain

$$\delta^{(3)} D_{ij}^{\pm}(t) = G_{11}(t)(t/\tau_u)^{-d} \sigma_{\mathrm{ff}}^2 \sigma_{\nu\nu}^2 (2\pi)^{d/2} \times \int_{k'} \widetilde{C}_{i1j1}(\mathbf{k}') \exp(-ik_1') + \cdots . \quad (29)$$

The function $G_{11}(t)$ is constant for $t \gg \tau_u$. Thus, the contribution due to $A_3^{\pm}(\mathbf{k}',t)$ scales as $(t/\tau_u)^{-d}$ and thus is subleading for $t \gg \tau_u$.

In summary, the leading-order terms of the dispersion coefficients are given by the steady-state contributions. For the longitudinal effective dispersion coefficient one obtains for $\epsilon \ll 1$ and $t \gg \tau_u$ [7],

$$D_{11}^{\mathrm{eff}}(t) = \sqrt{\frac{\pi}{2}} \sigma_{\mathrm{ff}}^2 u l [1 - (1 + 4t/\tau_D)^{-\frac{d-1}{2}}]. \quad (30)$$

The longitudinal ensemble dispersion coefficient in this limit is $D_{11}^{\mathrm{ens}} = \sqrt{\frac{\pi}{2}} \sigma_{\mathrm{ff}}^2 u l$. The transverse effective coefficients are of the order of the local dispersion coefficient D. The transverse ensemble coefficients behave as $(t/\tau_u)^{1-d}$.

We performed numerical random walk particle tracking simulations, which are based on the equivalence of the Fokker-Planck (3) and the Langevin equation,

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{u}[\mathbf{x}(t),t] + \sqrt{2D} \boldsymbol{\xi}(t), \quad (31)$$

with $\boldsymbol{\xi}$ a Gaussian white noise with zero mean and unit variance. The random fields $u_{il}'(\mathbf{x})$ in (4) are generated as (e.g., [8])

$$u_{i1}'(\mathbf{x}) = \sqrt{\frac{2\sigma_{\mathrm{ff}}^2}{N}} \sum_{i=1}^{N} p_{i1}(\mathbf{k}_i) \cos(\mathbf{k}_i \cdot \mathbf{x} + \phi_i), \quad (32)$$

where the $\mathbf{k}_i$ are independent Gaussian distributed random vectors with zero mean and variance $1/l^2$. The ϕ_i are independent and uniformly distributed in $[0,2\pi]$. The temporal random process $\nu(t)$ is generated as

$$\nu_1'(t) = \sqrt{\frac{2\sigma_{\nu\nu}^2}{N}} \sum_{i=1}^{N} \cos(\omega_i t + \varphi_i), \quad (33)$$

where the ω_i are independent Gaussian distributed random variables with zero mean and variance $1/\tau^2$. The φ_i are independent and uniformly distributed in $[0,2\pi]$. The fields are generated with $N = 64$. The random velocity field $\mathbf{u}(\mathbf{x},t)$ is constructed according to (4) for $\nu_i(t) = \delta_{i1}\nu_1(t)$. The simulations are performed using 10^4 realizations of the random velocity and 10^2 noise realizations per disorder realization. The Langevin equation is solved using an extended Runge-Kutta method (e.g., [9]) with $\Delta t = 10^{-1}$. The inverse Péclet number is $\epsilon = 10^{-2}$; the Kubo number is $\kappa = 1$.

The perturbation results derived in our paper are valid for a flow field of type (2). Thus, we performed numerical simulations also for transport in the velocity field given by

$$u_i(\mathbf{x},t) = u\delta_{i1} + u_{i1}'(\mathbf{x})\nu_1(t), \quad (34)$$

in order to demonstrate the validity of the analytical results obtained in our paper. The simulations use the same parameter values as above.

Figures 1 and 2 show the results of the numerical simulations and perturbation theory for the flow field (4) in $d = 2$ and $d = 3$ dimensions. The perturbation theory predictions are in good agreement with the numerical data. The behavior of the effective dispersion coefficients is essentially the same as the one found for dispersion in steady flow through a random medium.

Figures 3 and 4 compare the perturbation theory expressions (40) in our paper for longitudinal temporal fluctuations to simulations of dispersion in the flow field (34) in $d = 2$ and $d = 3$ dimensions. The numerical data are quite noisy, but it can be clearly seen that the perturbation theory expressions are in good agreement with the simulated effective dispersion coefficients.

In summary, we have presented corrections to the perturbation theory expressions for the effective and ensemble dispersion coefficients for transport in a temporally fluctuating flow field through a heterogeneous medium. We compared the corrected expressions to numerical random walk particle tracking simulations and found good agreement. We showed that the expressions for the dispersion coefficients given in our paper are consistent for flow fields that can be decomposed into a constant mean and a fluctuation whose space ensemble average is zero.

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