Erratum: Exact effective transport dynamics in a one-dimensional random environment [Phys. Rev. E **72**, 031110 (2005)]

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In our paper we derived an effective nonlocal equation for transport under random retardation properties based on a resummation of the perturbation series for the self-energy. Recently Dr. Victor P. Shkilev pointed out to us [1] that the expression for the self-energy obtained there was inconsistent. Here we provide consistent expressions for the self-energy and the resulting effective transport equations. The basic conclusions of our paper, namely, (i) on average, transport is described by a nonlocal equation whose kernel is uniquely determined by the disorder distribution, and (ii) the average description is equivalent to transport under linear kinetic adsorption and continuous time random walks, remain unchanged.

The total concentration $c(x,t)$ and the mobile concentration $c_m(x,t)$ for transport in a medium with random retardation properties are related by $c(x,t) = \theta(x)c_m(x,t)$, where the retardation coefficient $\theta(x) = 1 + k_d(x) > 1$ with $k_d(x)$ the distribution coefficient. It is modeled as a stationary random field.

Shkilev [1] remarked that the cumulative average total and mobile concentrations are related by

$$\int_0^\infty dt \overline{c}(x,t) = \overline{\theta} \int_0^\infty dt \overline{c}_m(x,t). \tag{1}$$

Furthermore, for narrow distributions of the retardation factor, the average total concentration can be approximated by $\overline{c}(x,t) = (1 + \overline{k}_d)\overline{c_m}(x,t)$.

Our paper derives a nonlocal equation for the ensemble average mobile concentration $\overline{c_m}(x,t)$ that is shown to be equivalent to transport under linear kinetic adsorption and continuous time random walks. The memory kernels that characterize these average transport models are uniquely defined in terms of the heterogeneity distribution. The expressions for the memory kernels and thus for the average behavior are expressed in terms of the self-energy $\Sigma(k,s)$. The latter is defined implicitly by

$$\overline{c}_m^*(k,s) = \frac{1}{\overline{\theta}s - ikq - \overline{\theta}\Sigma(k,s)}, \tag{2}$$

where $\widetilde{c}_m^*(k,s)$ denotes the Fourier-Laplace transform of $c_m(x,t)$. Furthermore, according to relation (28) in our paper the total concentration is given by

$$\overline{c}^*(k,s) = \overline{\theta}[1 - s^{-1}\Sigma(k,s)]\overline{c}_m^*(k,s). \tag{3}$$

The self-energy $\Sigma(k,s)$ is obtained in our paper based on a partial summation of the perturbation series for $\Sigma(k,s)$ and it is found that $\Sigma(k,s) = \Sigma(s)$ is independent of k. Thus, Eq. (2) implies directly a temporal nonlocal average transport equation for $\overline{c_m}(x,t)$. However, as noticed by Shkilev [1], the average expressions obtained are not consistent with relation (1).

Here we provide an alternative derivation that yields an exact expression for $\Sigma(k,s)$ and leads to explicit expressions for the average concentrations that are consistent with Eq. (1). Furthermore, the expression obtained below for $\Sigma(k,s)$ confirms that $\Sigma(k,s) = \Sigma(s)$ is independent of k. This implies that average transport is temporally nonlocal and uniquely defined in terms of the disorder distribution. Specifically, the nonlocal form of the governing equation for the average mobile concentration $\overline{c_m}(x,t)$,

$$\frac{\partial \overline{c_m}(x,t)}{\partial t} + \frac{\partial}{\partial t} \int_0^t dt' \, \phi(t-t')c(x,t') + \left[q\frac{\partial}{\partial x} - D\frac{\partial^2}{\partial x^2} \right]\overline{c_m}(x,t) = 0, \tag{4}$$

is unchanged, compare Eq. (58) in our paper. The specific form of the memory function $\phi(t)$, however, is different. The correct memory function is derived below and given in terms of its Laplace transform by Eq. (14). Furthermore, we demonstrate that the average transport model (4) is equivalent to linear kinetic adsorption and continuous time random walks also for the new memory function (14). As such, the main conclusions of our paper remain unchanged.

The starting point of our derivation is the transport equation for the mobile concentration,

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$$\theta(x)\frac{\partial c_m(x,t)}{\partial t} + q\frac{\partial c_m(x,t)}{\partial x} = 0, \tag{5}$$

where q is the constant flow velocity. Local dispersion is disregarded. The initial condition for $c_m(x,t)$ is $\theta(x)c_m(x,t{=}0)$ $=\delta(x)$. As boundary conditions we specify zero concentration at plus and minus infinity. Laplace transform (e.g., [2]) of Eq. (5) then gives

$$s\theta(x)c_m^*(x,s) + q\frac{\partial c_m^*(x,s)}{\partial x} = \delta(x). \tag{6}$$

The latter can be solved by separation of variables,

$$c_m^*(x,s) = q^{-1}\exp\left[-sq^{-1}\int_0^x dx'\,\theta(x')\right]H(x), \tag{7}$$

where $H(x)$ is the Heaviside step function. Using this expression one can already deduce Eq. (1). The Fourier transform of $c_m^*(x,s)$ is defined by

$$\tilde{c}^*(k,s) = \int_0^\infty \frac{dx}{q}\exp(ikx)\exp\left[-sq^{-1}\int_0^x dx'\,\theta(x')\right]. \tag{8}$$

We now coarse grain the resolution scale by defining $x=nl$, where l is large enough so that $\theta(x)$ and $\theta(x+l)$ can be considered uncorrelated, that is, it is of the order of the correlation scale of $\theta(x)$. We then obtain for $\tilde{c}_m^*(k,s)$

$$\tilde{c}_m^*(k,s) = \tau_q\sum_{n=0}^\infty \exp(iknl)\exp\left(-s\tau_q\sum_{j=0}^n \theta_j\right), \tag{9}$$

where we defined the advection time scale $\tau_q = l/q$.

The single point probability density function of $\theta(x)$ is given by $\overline{\delta[\theta-\theta(x)]} = \mathcal{P}(\theta)$. Thus, taking the ensemble average in Eq. (9), gives for $\overline{\tilde{c}_m^*}(k,s)$

$$\overline{\tilde{c}_m^*}(k,s) = \tau_q\sum_{n=0}^\infty \exp(iknl)\mathcal{P}^*(s\tau_q)^{n+1}. \tag{10}$$

The right side can be summed up to

$$\overline{\tilde{c}_m^*}(k,s) = \frac{\tau_q\mathcal{P}^*(s\tau_q)}{1 - \mathcal{P}^*(s\tau_q)\exp(ikl)}. \tag{11}$$

By comparison of Eq. (2) with Eq. (11), we find for the self-energy $\Sigma(k,s)\equiv\Sigma(s)$

$$\Sigma(s) = \frac{(1 + s\tau_q\bar{\theta})\mathcal{P}^*(s\tau_q) - 1}{\tau_q\bar{\theta}\mathcal{P}^*(s\tau_q)}, \tag{12}$$

where we disregard terms of order l. This expression is different from the one obtained in our paper by (partial) resummation of the perturbation series. Comparison of Eq. (12) with expression (53) in our paper reveals the terms that are disregarded in the partial resummation of the perturbation series.

(a) Effective equation: From expression (11), we obtain for $\overline{c_m^*}(x,s)$

$$sc_m^*(x,s)[1 + \phi^*(s)] = \frac{\overline{c_m^*}(x-l,s) - \overline{c_m^*}(x,s)}{\tau_q} + \delta(x), \tag{13}$$

where we defined the memory function

$$\phi^*(s) = \frac{1 - (1 + s\tau_q)\mathcal{P}^*(s\tau_q)}{s\tau_q\mathcal{P}^*(s\tau_q)}. \tag{14}$$

The average total concentration (3) now is given by

$$\overline{c^*}(x,s) = [1 + \phi^*(s)]\overline{c_m^*}(x,s). \tag{15}$$

Note that the memory function $\varphi^*(s)$ defined by Eq. (56) in our paper reads in terms of $\phi^*(s)$ as $\varphi^*(s) = [1 + \phi^*(s)]/\bar{\theta} - 1$.

By Taylor expansion of $\overline{c_m^*}(x-l,s)$ in Eq. (13) up to second order, we obtain the effective equation

$$s\overline{c_m^*}(x,s)[1 + \phi^*(s)] + \left[q\frac{\partial}{\partial x} - D\frac{\partial^2}{\partial x^2} \right]\overline{c_m^*}(x,s) = \delta(x),\tag{16}$$

where we defined $D = lq/2$. Its inverse Laplace transform is given by Eq. (4).

(b) Equivalence to linear kinetic adsorption models: Equation (16) describes transport under linear kinetic sorption characterized by the distribution of sorption time scale $P_{ad}(\tau)$. In this context, the memory function can be written as

$$\phi^*(s) = \bar{k}_d \int_0^\infty d\tau \frac{P_{ad}(\tau)}{1 + s\tau},\tag{17}$$

where $\bar{k}_d = \bar{\theta} - 1$. The distribution of adsorption time scales $P_{ad}(\tau)$ is characterized by its moments $m_\tau^{(n)}$, which are given in terms of the moments $m_\theta^{(k)}$ of $\theta(x)$ by the recursion relation (for $n > 0$)

$$m_\tau^{(n)} = \frac{m_\theta^{(n+1)}\tau_q^n}{\bar{k}_d(n+1)!} - \frac{m_\theta^{(n)}\tau_q^n}{\bar{k}_d n!} - \sum_{j=1}^n \frac{m_\theta^{(j)}\tau_q^j}{j!}m_\tau^{(n-j)}.\tag{18}$$

The average total concentration (15) in this picture is given by

$$\bar{c}(x,t) = \overline{c_m}(x,t) + \bar{k}_d \int_0^t dt' \int_0^\infty d\tau P_{ad}(\tau)\exp\left[-\frac{t-t'}{\tau} \right]\overline{c_m}(x,t').\tag{19}$$

If the distribution of adsorption times $P_{ad}(\tau)$ is narrow, that is, if it decays rapidly for $\tau \gg \tau_c$, with τ_c a characteristic time scale, then the latter expression can be approximated for $t \gg \tau_c$ by

$$\bar{c}(x,t) = (1 + \bar{k}_d)\overline{c_m}(x,t).\tag{20}$$

As outlined above, this relation was indicated as a consistence test for the upscaled result.

(c) Equivalence to continuous time random walks: The effective equation (21) reads in terms of the total concentration (15) as

$$s\overline{c^*}(x,s) + \left[q\frac{\partial}{\partial x} - D\frac{\partial^2}{\partial x^2} \right]\frac{s\tau_q\mathcal{P}^*(s\tau_q)}{1 - \mathcal{P}^*(s\tau_q)}\overline{c^*}(x,s) = \delta(x).\tag{21}$$

Comparison to the transport equation for the particle density of a continuous time random walk, see, e.g., Eq. (91) in our paper establishes immediately a relation between the distribution of retardation coefficients and the distribution of transition times $\psi(t)$, see also [3],

$$\psi(t) = \tau_q^{-1}\mathcal{P}(t/\tau_q).\tag{22}$$

In Ref. [3], these results are generalized for multiple dimensions and finite local scale dispersion using a Lagrangian upscaling approach.

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[1] V. P. Shkilev (private communication).

[2] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover Publications, New York, 1972).

[3] M. Dentz and A. Castro, Geophys. Res. Lett. **36**, L03403 (2009).