 Fluid reactive anomalous transport with random waiting time depending on the preceding jump length

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Anomalous (or non-Fickian) diffusion has been widely found in fluid reactive transport and the traditional advection diffusion reaction equation based on Fickian diffusion is proved to be inadequate to predict this anomalous transport of the reactive particle in flows. To capture the complex couple effect among advection, diffusion and reaction, and the energy-dependent characteristics of fluid reactive anomalous transport, in the present paper we analyze $A \rightarrow B$ reaction under anomalous diffusion with waiting time depending on the preceding jump length in linear flows, and derive the corresponding master equations in Fourier-Laplace space for the distribution of A and B particles in continuous time random walks scheme. As examples, the generalized advection diffusion reaction equations for the jump length of Gaussian distribution and lévy flight with the probability density function of waiting time being quadratic dependent on the preceding jump length are obtained by applying the derived master equations.

Keywords: Anomalous (or non-Fickian) diffusion, Continuous time random walk, Advection diffusion reaction equation

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1. Introduction

Fluid reactive transport is an important field of study in hydrogeology and other sciences that has a variety of applications such as the transport of contaminants in underground water$^{[1]}$, nuclear waste storage$^{[2]}$, and carbon dioxide ($CO_2$) storage$^{[2]}$, etc. The macroscopic description
of coupled reaction and transport is the standard advection diffusion reaction equation (ADRE) based on Fickian diffusion in one-dimensional form as:

$$\frac{\partial C(x,t)}{\partial t} + v \frac{\partial C(x,t)}{\partial x} = K \frac{\partial^2 C(x,t)}{\partial x^2} + f$$  \hspace{1cm} (1)$$

where $C(x,t)$ is the probability density function (PDF) of the particle, $v$ is constant velocity, $K$ is diffusion coefficient, and $f$ denotes the decoupled reaction term.

However, in recent years many tracer tests in natural complex porous media are found to exhibit anomalous diffusion (non-Fickian) behavior deviating from Fickian diffusion, and even without reaction ($f = 0$ in Eq.(1)) the classical advection-dispersion equation (ADE) has proven to be unsuitable for describing this kind of tracer transport.[2–6] One of the effective ways to quantify anomalous (or non-Fickian) transport in nonhomogeneous porous media is power law waiting time continuous time random walks (CTRW’s) model.[7–9] Based on various CTRW models scholars obtain several generalization types of ADE which can be used to describe the evolution of the probability density function (PDF) of the particles undergoing anomalous dispersion in flow fields.[10–11]

On the other hand, there are some reaction-anomalous diffusion equations where the reaction term has nontrivial coupled effect on diffusion term proposed.[12–16] More recently a modified fractional ADRE,

$$\frac{\partial C_m(x,t)}{\partial t} + \frac{\partial^r C_m(x,t)}{\partial t^r} = K \frac{\partial^2 C_m(x,t)}{\partial x^2} - \frac{t^{-r}}{\Gamma(1-r)} C_{m,0}$$  \hspace{1cm} (2)$$

was derived for the transport of mobile concentration of upscaling chemical reactions in multi-continuum systems.[17] Eq.(2) convolves a memory function $\frac{t^{-r}}{\Gamma(1-r)}$ and the time derivative term, and shows that the description of the upscaling procedure in the presence of reactions is not a fractional diffusion equation with a naive reaction term added. It should be noted that for the sake of simplicity in the above transport equation the drift (advection) term is not included, and is considered to be relatively straightforward. But in fact, the advection term may have a complex coupled effect on the anomalous diffusion and the chemical reaction terms in some circumstances[9,18], and should be further considered.

In 2006, Zaburdaev proposed a generalized CTRW model for certain circumstances in which the waiting time is connected with the preceding jump length. This model describes the dependence of the random waiting time on the energy and suggests a method that includes the details of the microscopic distribution over the waiting times and arrival distances at a given
Note that up to now this coupled CTRW model has been not associated with the fluid reactive transport. In the present paper we shall consider the simple A→B reaction under anomalous diffusion on moving fluid based on this CTRW model with random waiting time depending on the preceding jump length, which can not only show the coupling among advection velocity, anomalous diffusion and chemical reaction, but also describe the energy-dependent characteristics of fluid reactive anomalous transport. As examples, we shall apply the new master equation to derive four generalized ADRE’s for Gaussian distribution and lévy flight for jump lengths in linear flows when the microscopic distribution of the random sojourn time is quadratic dependent on the preceding jump length.

2. Coupled CTRW model with random waiting time depending on the preceding jump length

We first recall the coupled CTRW model with waiting time depending on the spent energy or the preceding jump length in one-dimensional lattices proposed by Zaburdaev. In this model, each step of the particle requires some energy, and after making a jump a particle needs time to recover. The longer the preceding jump distance, the longer are the recovery and the waiting time. It means that the PDF of the waiting time $\psi(|y|, t)$ before making the second step depends both on the length of the preceding jump $|y|$ and the waiting time $t$. Thus, the particle jumps from $x - y$ to $x$ with the jump length PDF $\lambda(y)$, and then waits at $x$ for time $t$ drawn from $\psi(|y|, t)$, after which the process is renewed. By assuming that in the initial state all particles have zero arrival distances and zero resting times, one obtained the balance equation for the PDF $\rho(x, t)$ of the particles

$$\rho(x, t) = \int_{-\infty}^{+\infty} dx' \int_0^t j(x', t') \lambda(x - x') \Psi(|x - x'|, t - t') dt' + \Psi_0(t) \rho_0(x).$$

(3)

Here, $j(x, t)$ is the escape rate, and satisfies the equation

$$j(x, t) = \int_{-\infty}^{+\infty} dx' \int_0^t j(x', t') \lambda(x - x') \psi(|x - x'|, t - t') dt' + \psi_0(t) \rho_0(x),$$

(4)

where the survival time distribution $\Psi(|y|, t) = 1 - \int_0^t \psi(|y|, \tau) d\tau$ depends both on the waiting time and the preceding jump length, the term $\Psi_0(t) \rho_0(x) = \Psi(|0|, t) \rho(x, 0)$ is supposed as the influence of the initial distribution, and $\psi_0(t) = \psi(|0|, t)$ is the waiting time PDF for the initial
position. In Fourier-Laplace space, the PDF $\rho(x, t)$ obeys the master equation for the CTRW model with waiting time depending on the preceding jump length:

$$\rho(k, u) = \Psi(u)\rho_0(k) + \frac{\{\Psi(|x|, u)\lambda(x)\}k\psi(u)}{1 - \{\psi(|x|, u)\lambda(x)\}k},$$

(5)

where the symbol $\psi(u)$ is the Laplace transform of $\psi_0(t)$, and $\Psi(u)\rho_0(k)$, $\{\Psi(|x|, u)\lambda(x)\}k$, $\{\psi(|x|, u)\lambda(x)\}k$ denote the Fourier-Laplace transform of $\Psi_{0}(t)\rho_{0}(x)$, $\Psi(|x|, t)\lambda(x)$, $\psi(|x|, t)\lambda(x)$, respectively.

3. Fluid reactive anomalous transport with random waiting time depending on the preceding jump length

We shall now consider the energy dependent random walk model in a moving fluid with an inhomogeneous velocity field $v(x)$. Noting that in Ref.[9], [10] and [20] in Galilei variant model the jump length $y$ for the moving particle dragged along the velocity $v(x)$ is replaced by $y - \tau_a v(x)$, where $\tau_a$ stands for an advection time scale, and $\tau_a v(x)$ is the mean drag experienced by a particle jumping from the point $x$, in our model we introduce the PDF of a length of step $y$ with waiting time $t$ which will depend on the velocity $v(x)$ of the fluid with the starting point $x$ of the jump, i.e., $\lambda(y - \tau_a v(x))\Psi(|y - \tau_a v(x)|, t)$. When $v(x) = 0$, this PDF recovers the coupled density $\lambda(y)\Psi(|y|, t)$ for the particle in Ref. [19].

We then study the simplest reaction scheme $A \rightarrow B$ in this CTRW model. We assume all physical properties of A and B particles are the same and the particles trapped in stagnant regions will react with a relabeling of A into B taking place at a rate $\alpha$ without changing energy. Let $A(x, t)$ be the PDF of A particle being in point $x$ at time $t$ and and $i^-(x, t)$ be the escape rate. By assuming that in the initial distribution all particles have zero resting times, we can find the balance equation for A particles in a given point:

$$A(x, t) = A_0(x)\Psi_0(t)e^{-\alpha t} + \int_{-\infty}^{+\infty} dx' \int_{0}^{t} i^-(x', t')\lambda(x - x' - \tau_a v(x'))$$

$$\times\Psi(|x - x' - \tau_a v(x')|, t - t')e^{-\alpha(t-t')} dt'$$

(6)

where $A_0(x)$ is the initial state of A particle, $\Psi(|y|, t)e^{-\alpha t} = (1 - \int_{0}^{t} \psi(|y|, \tau)d\tau)e^{-\alpha t}$ is the joint survival density of remaining at least at time $t$ on the spot (without being converted into B). The density is a sum of outgoing particles from all other points at different times given by the
flow, and provided they survived after their arrival till the time \( t \). The first term on the right hand side is just the influence of the initial distribution.

Fourier transforming \( x \to k \) and Laplace transforming \( t \to u \) of Eq.\((\ref{eq:7})\), we find

\[
A(k, u) = A_0(k)\Psi_0(u + \alpha) + \left[\Psi(i\frac{\partial}{\partial k}, u + \alpha)\lambda(k)\right]\int_{-\infty}^{+\infty} i^-(x', u)e^{-k(x' + \tau_0v(x'))}dx'. \tag{7}
\]

In the above expression \( A_0(k) \) represents the Fourier \( x \to k \) transform of the initial condition \( A_0(x) \), \( \Psi_0(u + \alpha) \) denotes the Laplace transform of joint survival PDF \( \Psi_0(t)e^{-\alpha t} \), \( A(k, u) \) and \( i^-(k, u) \) are the Fourier-Laplace transforms of \( A(x, t) \) and \( i^-(x, t) \) respectively, and the term \( \Psi(i\frac{\partial}{\partial k}, u + \alpha)\lambda(k) \) represents the Fourier-Laplace transform of \( \Psi(|x|, t)\lambda(x) \) where we use the property of Fourier transform \( \mathcal{F}(xf(x)) = i\frac{\partial}{\partial k}f(k) \).

To get the master equation with respect to \( A(x, t) \), we shall give the other balance equation. We notice that that the loss flux is from those particles that were originally at \( x \) at \( t = 0 \) and wait without reacting until time \( t \) to leave, and those particles that arrived at an earlier time \( t' \) and wait without reacting until time \( t \) to leave, and have the second balance equation:

\[
i^-(x, t) = A_0(x)\psi_0(t)e^{-\alpha_1 t} + \int_{-\infty}^{+\infty} dx' \int_0^t \lambda(x - x' - \tau_0v(x')) \psi(|x - x' - \tau_0v(x')|, t - t')e^{-\alpha(t - t')} dt'
\tag{8}
\]

where \( \psi(|x - x'|, t - t')e^{-\alpha(t - t')} \) is the non-proper waiting time density depending on the preceding jump length for the actually made new step provided the particle survived. By applying the transform \( (x, t) \to (k, u) \) of Eq.\(\ref{eq:7}\), we find

\[
i^-(k, u) = A_0(k)\psi_0(u + \alpha) + \left[\psi(i\frac{\partial}{\partial k}, u + \alpha)\lambda(k)\right]\int_{-\infty}^{+\infty} i^-(x', u)e^{-k(x' + \tau_0v(x'))}dx'. \tag{9}
\]

where the term \( \psi(i\frac{\partial}{\partial k}, u + \alpha)\lambda(k) \) is the Fourier-Laplace transform of \( \Psi(|x|, t)\lambda(x) \). Using \(\ref{eq:7}\) and \(\ref{eq:9}\), one has

\[
\frac{A(k, u) - A_0(k)\Psi_0(u + \alpha)}{\Psi(i\frac{\partial}{\partial k}, u + \alpha)\lambda(k)} = \frac{i^-(k, u) - A_0(k)\psi_0(u + \alpha)}{\psi(i\frac{\partial}{\partial k}, u + \alpha)\lambda(k)}, \tag{10}
\]

from which we find

\[
i^-(k, u) = A_0(k)\psi_0(u + \alpha) + \psi(i\frac{\partial}{\partial k}, u + \alpha)\lambda(k)A(k, u) - A_0(k)\Psi_0(u + \alpha). \tag{11}
\]

We assume a linear velocity \( v(x) = \omega x \) where \( \omega \) is a constant. Then Eq.\(\ref{eq:7}\) becomes

\[
A(k, u) = \Psi(u + \alpha)A_0(k) + \psi(i\frac{\partial}{\partial k}, u + \alpha)\lambda(k)j(k + v_k, u) \tag{12}
\]
where the symbol $v_k = \tau_0 \omega k$. In the limit $\tau_a \to 0$, Eq. (12) gives

$$A(k, u) \simeq \Psi(u + \alpha) A_0(k) + \Psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k) \times [i^-(k, u) + v_k i^{-'}(k, u)]. \quad (13)$$

We substitute (11) into (13) and finally obtain the generalized master equation in Fourier-Laplace space for the distribution of $A$-particles in $A \to B$ reaction-anomalous diffusion in fluid fields with waiting time depending the preceding jump length:

$$\mathcal{D}(k, u) A(k, u) = \mathcal{V}(k, u) A'_0(k, u) + \mathcal{I}(k, u) \quad (14)$$

where

$$\mathcal{D}(k, u) = [1 - \psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)] - v_k \Phi_\alpha(k, u) [\Psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)],$$

$$\mathcal{V}(k, u) = v_k [\psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)],$$

$$\mathcal{I}(k, u) = -v_k [\Psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)] \Phi_\alpha(k, u) \Psi_0(u + \alpha) A_0(k)$$

$$+ [1 - \psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)] \Psi_0(u + \alpha) A_0(k) + v_k [\Psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)] \psi_0(u + \alpha) A'_0(k)$$

$$- v_k [\psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)] \Psi_0(u + \alpha) A'_0(k) + [\Psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)] \psi_0(u + \alpha) A_0(k),$$

where $\Phi_\alpha(k, u) = \frac{\psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)}{\Psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)}$, and the term $\mathcal{I}(k, u)$ denotes the influence of the initial condition. One can see that in above master equation advection and diffusion terms are coupled, and both depend on the reaction rate $\alpha$. When the reaction rate $\alpha = 0$, Eq. (14) reduces to the master equation for CTRW in flows with the waiting time depending on the preceding jump length in nonreactive system derived in Ref. [9]. Note also that for $\tau_a \to 0$, Eq. (9) gives

$$i^-(k, u) \simeq [\psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)] [i^-(k, u) + v_k i^{-'}(k, u)] + \psi_0(u + \alpha) A_0(k). \quad (15)$$

Substituting (11) into (15), we can also find Eq. (14).

Analogously we shall now study the transport for the $B$-particles in $A \to B$ reaction under energy-dependent anomalous diffusion in fluid fields. Let $B(x, t)$ be the PDF of $B$ particle being in point $x$ at time $t$, $j^+(x, t)$ be the gain flux and $j^-(x, t)$ be the loss flux of particles $B$ at site $x$ at $t$. Noting that $B$-particle that is at (or leaves) site $x$ at time $t$ either has come there as a $B$-particle at some prior time or was converted from an $A$-particle that either was on site $x$
from the very beginning or arrived there later at \( t' > 0 \) while keeping the same energy, and still stays (or just leaves) the site \( x \) at time \( t \), we give the following balance equations:

\[
B(x, t) = \int_{-\infty}^{+\infty} dx' \int_0^t j^-(x', t') \lambda(x - x' - \tau_a v(x')) |\Psi(|x - x' - \tau_a v(x')|, t - t')| dt' \\
+ \int_{-\infty}^{+\infty} dx' \int_0^t i^-(x', t') \lambda(x - x' - \tau_a v(x')) |\Psi(|x - x' - \tau_a v(x')|, t - t')| dt' \\
\times (1 - e^{-\alpha(t-t')}) dt' + A_0(x) \Psi_0(t)(1 - e^{-\alpha t}),
\]

(16)

and

\[
\dot{j}^-(x, t) = \int_{-\infty}^{+\infty} dx' \int_0^t j^-(x', t') \lambda(x - x' - \tau_a v(x')) |\psi(|x - x' - \tau_a v(x')|, t - t')| dt' \\
+ \int_{-\infty}^{+\infty} dx' \int_0^t i^-(x', t') \lambda(x - x' - \tau_a v(x')) |\psi(|x - x' - \tau_a v(x')|, t - t')| dt' \\
\times (1 - e^{-\alpha(t-t')}) dt' + A_0(x) \dot{\psi}_0(t)(1 - e^{-\alpha t}),
\]

(17)

where the initial condition \( B_0(x) = 0 \) was used. Laplace \( x \rightarrow k \) and Fourier \( t \rightarrow u \) transforming of the two equations (16) and (17) yields:

\[
B(k, u) = [\Psi(i \frac{\partial}{\partial k}, u) \lambda(k)] \int_{-\infty}^{+\infty} j^-(x', u) e^{-k(x'+\tau_a v(x'))} dx' + [\Psi(i \frac{\partial}{\partial k}, u) \lambda(k) - \Psi(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)] \\
\times \int_{-\infty}^{+\infty} i^-(x', u) e^{-k(x'+\tau_a v(x'))} dx' + A_0(k) [\Psi_0(u) - \Psi_0(u + \alpha)],
\]

(18)

and

\[
\dot{j}^-(k, u) = [\dot{\psi}(i \frac{\partial}{\partial k}, u) \lambda(k)] \int_{-\infty}^{+\infty} j^-(x', u) e^{-k(x'+\tau_a v(x'))} dx' + [\dot{\psi}(i \frac{\partial}{\partial k}, u) \lambda(k) - \dot{\psi}(i \frac{\partial}{\partial k}, u + \alpha) \lambda(k)] \\
\times \int_{-\infty}^{+\infty} i^-(x', u) e^{-k(x'+\tau_a v(x'))} dx' + A_0(k) [\dot{\psi}_0(u) - \dot{\psi}_0(u + \alpha)].
\]

(19)

Here, \( B(k, u) \) and \( \dot{j}^-(k, u) \) are the Fourier-Laplace transforms of \( B(x, t) \) and \( \dot{j}^-(x, t) \), respectively.

Comparing (7), (9), (18) and (19), one has

\[
\frac{A(k, u) + B(k, u) - A_0(k) \Psi_0(u)}{\Psi(i \frac{\partial}{\partial k}, u) \lambda(k)} = \frac{i^- (k, u) + j^- (k, u) - A_0(k) \dot{\psi}_0(u)}{\dot{\psi}(i \frac{\partial}{\partial k}, u) \lambda(k)},
\]

(20)

from which we find

\[
\dot{j}^-(k, u) = A_0(k) \dot{\psi}_0(u) - i^-(k, u) + \Phi_0(k, u) [A(k, u) + B(k, u) - A_0(k) \Psi_0(u)].
\]

(21)

To get the master equation for \( B(k, u) \), we consider the third balance equation\(^{12}\):

\[
\frac{\partial B(x, t)}{\partial t} = j^+(x, t) - j^-(x, t) + \alpha A(x, t).
\]

(22)
Here, $j^+(x, t)$ is the gain flux which can be represented by the loss flux$^{[21]}

\[ j^+(x, t) = \int_{-\infty}^{+\infty} j^-(x', t) \lambda(x - x' - \tau_a v(x')) dx'. \quad (23) \]

Transforming $(x, t) \rightarrow (k, u)$ of (22) yields

\[ uB(k, u) = \lambda(k) \int_{-\infty}^{+\infty} j^-(x', u) e^{-k(x' + \tau_a v(x'))} dx' - j^-(k, u) + \alpha A(k, u), \quad (24) \]

Assuming $v(x) = \omega x$, in the limit $\tau_a \rightarrow 0$, we find

\[ uB(k, u) = (\lambda(k) - 1)j^-(k, u) + v_k \lambda(k)j^-(k, u) + \alpha A(k, u), \quad (25) \]

we substitute Eq.(21) into (25), and finally obtain the generalized master equation in Fourier-Laplace space for the distribution of B-particles in $A \rightarrow B$ reaction-anomalous diffusion on moving flows with waiting time depending the preceding jump length:

\[ D_1(k, u)B(k, u) + D_2(k, u)A(k, u) = V_1(k, u)B_k'(k, u) + V_2(k, u)A_k'(k, u)(k, u) + I(k, u) \quad (26) \]

where

\[ D_1(k, u) = u - (\lambda(k) - 1)\Phi_0(k, u) - \lambda(k)v_k \Phi_0(k, u)', \]

\[ D_2(k, u) = (1 - \lambda(k)) [\Phi_0(k, u) - \Phi_a(k, u)] + \lambda(k)v_k [\Phi_0(k, u)' - \Phi_a(k, u)'] - \alpha, \]

\[ V_1(k, u) = \lambda(k)v_k \Phi_0(k, u), \]

\[ V_2(k, u) = \lambda(k)v_k [\Phi_0(k, u) - \Phi_a(k, u)], \]

\[ I(k, u) = [\lambda(k) - 1]A_0(k) \{ [\psi_0(u) - \psi_0(u + \alpha)] - [\Phi_0(k, u)\Psi_0(u) - \Phi_a(k, u)\Psi_0(u + \alpha)] \}
+ \lambda(k)v_k [A_0'(k)[\psi_0(u) - \psi_0(u + \alpha)] - A_0'(k)[\Phi_0(k, u)\Psi_0(u) - \Phi_a(k, u)\Psi_0(u + \alpha)]
- A_0(k)[\Phi_0(k, u)'\Psi_0(u) - \Phi_a(k, u)'\Psi_0(u + \alpha)] \}

where the term $I(k, u)$ denotes the influence of the initial condition. Eq.(26) shows the complex coupled relations among diffusion, advection and reaction terms. The generalized ADRE's for B-particles can be derived from Eq.(20) by carrying out the macroscopic limit and inverting the Fourier-Laplace transform.
4. Examples and generalized ADRE’s

We now turn to apply the master equations (14) and (26) to derive the corresponding ADRE’s for A and B particles when the jump lengths obey Gaussian distribution or lévy flight and the waiting time PDF is quadratic dependent on the preceding jump length, i.e.,

\[ \psi(|y|, t) = \delta(t - \theta y^2), \]  

(27)

where the length-dependent parameter \( \theta > 0 \).

We first consider the case for Gaussian jump length PDF

\[ \lambda(y) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{y^2}{2\sigma^2}}. \]  

(28)

Then, the corresponding Laplace and Fourier transforms of \( \psi(|y|, t), \lambda(y) \) become

\[ \psi(|y|, u) = e^{-\theta y^2 u} \sim 1 - \theta y^2 u, \]

(29)

\[ \lambda(k) = e^{-\frac{\sigma^2 k^2}{2}} \sim 1 - \frac{\sigma^2 k^2}{2}, \]

(30)

from which we find

\[ \psi(i \frac{\partial}{\partial k}, u) \lambda(k) = 1 - \frac{\sigma^2 k^2}{2} - \theta \mu \sigma^2, \]

(31)

\[ \Psi(i \frac{\partial}{\partial k}, u) \lambda(k) = \theta \sigma^2. \]

(32)

Assuming \( A_0(x) = \delta(x) \), substituting Eq.(31) and (32) and the initial condition \( \psi_0(u) = 1, \Psi_0(u) = 0 \) into Eq.(14), in the limit of \( \tau_a \to 0 \) and \( \sigma \to 0 \) we obtain

\[ \left( \frac{k^2}{2\theta} + u + \alpha \right) A(k, u) = \frac{A}{\theta} \omega k \rho_k'(k, u) + 1 \]

(33)

Inverting Eq.(33) to the space-time domain \( k \to x \) and \( s \to t \), we then get the generalized ADRE for A-particles with energy-dependent parameter:

\[ \hat{T}_t(1, \alpha) A(x, t) + \frac{A \partial (v(x) A(x, t))}{\partial x} = \frac{1}{2\theta} \frac{\partial^2 A(x, t)}{\partial x^2} \]

(34)

with the initial condition \( A_0(x) = \delta(x) \). Here, The integral operator \( \hat{T}_t(1 - \beta, \alpha) f = \tau^\beta \Gamma(1 - \beta) \int_0^t \Phi(t') f(t') dt' \) corresponds in time domain to

\[ \hat{T}_t(1 - \beta, \alpha) f = \frac{d}{dt} \int_0^t e^{-\alpha(t-t')} (t-t')^{1-\beta} f(t') dt' + \alpha \int_0^t e^{-\alpha(t-t')} (t-t')^{1-\beta} f(t') dt' \]

(35)
and becomes a fractional derivative when $\alpha = 0$ \cite{12}. One can see that in the generalized ADRE (35) the diffusion operate depend on reaction rate $\alpha$, and the advection and diffusion coefficients include the length-dependent parameter $\theta$.

If we substitute Eq.\,(31) and (32) and the initial condition $B_0(x) = 0$, $\psi_0(u) = 1$, $\Psi_0(u) = 0$ into Eq.(26), in the limit of $\tau_a \rightarrow 0$ and $\sigma \rightarrow 0$, we then find

$$\frac{k^2}{2\theta} B(k,u) = \frac{A}{\theta} \omega B'(k,u) + \alpha A(k,u)$$  \hspace{1cm} (36)

Inverting Eq.(36) to the space-time domain , we obtain the generalized ADRE for B-particles:

$$\frac{\partial B(x,t)}{\partial t} + \frac{A}{\theta} \frac{\partial (v(x)B(x,t))}{\partial x} = \frac{1}{2\theta} \frac{\partial^2 B(x,t)}{\partial x^2} + \alpha A(x,t)$$  \hspace{1cm} (37)

with the initial condition $B_0(x) = 0$. Note that the advection and diffusion coefficients depend on the length-dependent parameter $\theta$.

Secondly, we choose a Lévy distribution for the jump length, i.e.,

$$\lambda(k) = e^{-\frac{1}{2}\frac{\sigma^\beta k^\beta}{\beta}} \sim 1 - \frac{1}{2} \sigma^\beta k^\beta$$  \hspace{1cm} (38)

with $1 < \beta \leq 2$. Thus, for the length-dependent waiting time PDF

$$\psi(|y|,t) = \delta(t - \theta y^2), \theta > 0,$$

we have

$$\psi(i \frac{\partial}{\partial k}, u) \lambda(k) = 1 - \frac{1}{2} \sigma^\beta k^\beta - \frac{1}{2} \theta u \sigma^\beta (\beta - 1) k^{\beta - 2},$$  \hspace{1cm} (39)

$$\Psi(i \frac{\partial}{\partial k}, u) \lambda(k) = \frac{1}{2} \theta \sigma^\beta (\beta - 1) k^{\beta - 2}.$$  \hspace{1cm} (40)

For the initial condition $\rho_0(x) = \delta(x)$, in the limit of small $\tau_a$ and $\sigma$, Eq.\,(14) then becomes

$$\left(\frac{1}{\theta \beta (\beta - 1)} k^2 + u + \alpha\right) A(k,u) = \frac{2}{\theta \beta (\beta - 1)} \omega k^{3-\beta} A'(k,u) + 1,$$  \hspace{1cm} (41)

where $A = \lim_{\tau_a \rightarrow 0, \sigma \rightarrow 0} \frac{\sigma^\beta}{\sigma^\beta} \theta$ is kept finite. The inverse Fourier-Laplace transform of Eq.(30) leads to the generalized fractional ADRE for A-particles:

$$\hat{T}(1, \alpha) A(x,t) = \frac{2 A i^\beta}{\theta \beta (\beta - 1)} D^{3-\beta}_x (v(x)A(x,t)) = \frac{1}{\theta \beta (\beta - 1)} \frac{\partial^2 A(x,t)}{\partial x^2}$$  \hspace{1cm} (42)

with the initial condition $\rho_0(x) = \delta(x)$. Here, the operator $D^{3-\beta}_x$ is the fractional derivative of the Riemann-Liouville type,\cite{22} equal in Fourier $x \rightarrow k$ space to $(ik)^{3-\beta}$. In (42) the advection
and diffusion coefficients both involve the length-dependent parameter \( \theta \). Note also that this generalized fractional equation (42) reduces to Eq.(34) when \( \beta = 2 \).

Analogously for \( B_0(x) = 0 \), in the limit of small \( \tau_a \) and \( \sigma \), Eq.(26) becomes

\[
\frac{1}{\theta \beta (\beta - 1)} k^2 + u) B(k, u) = A \frac{2}{\theta \beta (\beta - 1)} \omega k^{3-\beta} B'_k(k, u) + \alpha A(k, u),
\]

(43)

Inversing Eq.(43), we obtain the generalized fractional ADRE for B-particles with energy-dependent parameter \( \theta \):

\[
\frac{\partial B(x, t)}{\partial t} - \frac{2 A i^\beta}{\theta \beta (\beta - 1)} D^{3-\beta}_x (v(x) B(x, t)) = \frac{1}{\theta \beta (\beta - 1)} \frac{\partial^2 B(x, t)}{\partial x^2} + \alpha A(x, t).
\]

(44)

If \( \beta = 2 \), this generalized fractional equation then reduces to Eq.(37).

Finally, assume that \( C(x, t) \) is the sum of \( A(x, t) \) and \( B(x, t) \), and combine (34) with (37), and we have

\[
\frac{\partial C(x, t)}{\partial t} + A \frac{\partial (v(x) C(x, t))}{\partial x} = \frac{1}{2\theta} \frac{\partial^2 C(x, t)}{\partial x^2}.
\]

(45)

From (42) and (44), one has

\[
\frac{\partial C(x, t)}{\partial t} - \frac{2 A i^\beta}{\theta \beta (\beta - 1)} D^{3-\beta}_x (v(x) C(x, t)) = \frac{1}{\theta \beta (\beta - 1)} \frac{\partial^2 C(x, t)}{\partial x^2}.
\]

(46)

Note that Eq.(45) and (46) are consistent with the generalized advection-dispersion equations with waiting time depending on the preceding jump length derived in Ref. [9] recently. Note also that in above two equation there are no reaction terms except diffusion terms. It is because that the \( A \rightarrow B \) reaction we discuss here does not change the sum of the particles in the reactive system.

5. Conclusions

To sum up, in this paper we derive the master equations (14) and (26) for the PDF of A and B particles in reaction \( A \rightarrow B \) under anomalous diffusion in linear flows with random waiting time depending on the preceding jump length based on the CTRW model. As examples, we obtain four generalized ADRE’s (32), (37), (42) and (44) for the probability density function of reactive particles by applying the derived master equations, and show the energy-dependent characteristics of the particles in fluid reactive anomalous transport. There are problems such as the energy-dependent behaviors for more complex reaction under anomalous diffusion on moving fluid are still unknown.
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