Reaction-subdiffusion in moving fluids

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To capture the dynamic behaviors of reaction-subdiffusion in linear flow fields, in the present paper we analyze a simple monomolecular conversion $A \to B$. We derive the corresponding master equations for the distribution of A and B particles in continuous time random walk schemes. The results are then used to obtain the generalizations of the advection-diffusion reaction equation in which the diffusion and advection operators both depend on the reaction rate.

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I. INTRODUCTION

Reactive transport in flows is an important issue of diffusion theory that has a variety of applications in many topics, such as the transport of contaminants in underground water [1], nuclear waste storage [2], etc. The macroscopic description of reaction-diffusion in a velocity field is the standard advection-diffusion reaction equation (ADRE) defined in one-dimensional form as

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

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

In recent years the reaction under anomalous diffusion has attracted more and more attentions [3]. One of the effective ways to capture anomalous diffusion is the continuous time random walk (CTRW) model [4–7]. By using the CTRW scheme Sokolov *et al.* analyzed the reaction-subdiffusion process for the monomolecular conversion $A \to B$, derived the corresponding kinetic equations for local A and B concentrations and first argued that reaction-subdiffusion equations are not obtained by a trivial change of the diffusion operator for a subdiffusion one [3]. Such a nontrivial coupled effect was also found in the multispecies system undergoing anomalous subdiffusion with linear reaction dynamics [8] and some other reaction-subdiffusion systems [9–12].

However, up to now few works have approached the reaction under anomalous diffusion in nonhomogeneous flows [13–15]. Without considering the effect of chemical reactions, Compte [16] and Compte *et al.* [17] have discussed anomalous diffusion in a nonhomogeneous convection velocity field by applying the CTRW techniques in which the step length distribution function depends on the starting point of the jump and showed that the convection coefficient depends on the waiting time statistics. The more basic and interesting problem of how nonhomogeneous velocity fields might affect the reaction under anomalous diffusion is attempted here. It is what we will address in this paper. In what follows we will consider the reaction-subdiffusion process on a linear moving fluid for the reaction $A \to B$ in the CTRW scheme then derive the generalizations of advection-diffusion reaction equation and show the interesting coupling relations between the velocity field and the chemical reactions under subdiffusion.

II. REACTION-SUBDIFFUSION IN FLOWS

A. CTRW scheme for A particles and corresponding ADRE

We start by recalling the CTRW model on inhomogeneous flows in the one-dimensional case [16,17]. In this model, the jump length y for the moving particle is dragged along the velocity $v(x)$ and replaced by $y - \tau_a v(x)$ where τ_a stands for an advection timescale and $\tau_a v(x)$ is the mean drag experienced by a particle jumping from point x. Thus, the particle jumps from x to $x + y$ with the jump length PDF $\lambda[y - \tau_a v(x)]$ and then waits at $x + y$ for time t drawn from $\psi(t)$ after which the process is renewed.

We then consider the simplest reaction scheme $A \to B$ in this CTRW model. We assume all 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 α. Let $A(x,t)$ be the PDF of the 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 the A particles in a given point,

$$A(x,t) = A_0(x)\Psi(t)e^{-\alpha t} + \int_{-\infty}^{+\infty} dx' \int_0^t i^-(x',t') \times \lambda[x - x' - \tau_a v(x')]\Psi(t-t')e^{-\alpha(t-t')}dt', \tag{2}$$

where $A_0(x)$ is the initial state of the A particle, $\Psi(t)e^{-\alpha t} = [1 - \int_0^t \psi(\tau)d\tau]e^{-\alpha t}$ 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 until time t. The first term on the right hand side is the influence of the initial distribution.

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The above equation (2) can be changed to the form

$$A(x,t) = A_0(x)\Psi(t)e^{-\alpha t} + \int_{-\infty}^{+\infty} dx' \int_0^t i^-(x',t') \times \phi(x-x',t-t';x')e^{-\alpha(t-t')}dt', \quad (3)$$

by using the expression $\phi(r,\tau;x) = \lambda[r-\tau_a v(x)]\Psi(\tau)$ [16]. Fourier transforming $x \to k$ and Laplace transforming $t \to u$ of Eq. (3), we obtain

$$A(k,u) = A_0(k)\Psi(u+\alpha) + \int i^-(k',u)\phi(k,u+\alpha;k-k')dk'. \quad (4)$$

Here, $A_0(k)$ represents the Fourier $x \to k$ transform of the initial condition $A_0(x)$, $\Psi(u+\alpha)$ denotes the Laplace transform of joint survival PDF $\Psi(t)e^{-\alpha t}$, $A(k,u)$, $i^-(k,u)$, respectively, are the Fourier-Laplace transforms of $A(x,t)$, $i^-(x,t)$, and

$$\phi(k,u+\alpha;k-k') = \Psi(u+\alpha)\lambda(k)\int e^{-ik\tau_a v(x')}e^{-i(k-k')x'}dx'. \quad (5)$$

To obtain the master equation with respect to $A(x,t)$, we will give the other balance equation. Noting 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, we have the second balance equation,

$$i^-(x,t) = A_0(x)\psi(t)e^{-\alpha t} + \int_{-\infty}^{+\infty} dx' \int_0^t i^-(x',t') \times \lambda[x-x'-\tau_a v(x')]\psi(t-t')e^{-\alpha(t-t')}dt', \quad (6)$$

where $\psi(t)e^{-\alpha t}$ is the nonproper waiting time density for the actually made new step provided the particle survived [3]. By introducing

$$\eta(r,\tau;x) = \lambda[r-\tau_a v(x)]\psi(\tau),$$

and applying the transform $(x,t) \to (k,u)$ of Eq. (6), we find

$$i^-(k,u) = A_0(k)\psi(u+\alpha) + \int i^-(k',u)\eta(k,u+\alpha;k-k')dk', \quad (7)$$

where the term,

$$\eta(k,u+\alpha;k-k') = \psi(u+\alpha)\lambda(k)\int e^{-ik\tau_a v(x')}e^{-i(k-k')x'}dx'.$$

We divide Eq. (4) by (7) to write

$$i^-(k,u) = \frac{\psi(u+\alpha)}{\Psi(u+\alpha)}A(k,u). \quad (8)$$

Noting that $\Psi(u+\alpha) = \frac{1-\psi(u+\alpha)}{u+\alpha}$, we get

$$i^-(k,u) = \Phi_\alpha(u)A(k,u), \quad (9)$$

where $\Phi_\alpha(u) = \frac{(u+\alpha)\psi(u+\alpha)}{1-\psi(u+\alpha)}$, which recovers the relation between $A(x,t)$ and $i^-(x,t)$ when the effect of the flow field is not considered in Ref. [3]. Inverting Eq. (9) to the space-time domain $k \to x$, $s \to t$, we obtain

$$i^-(x,t) = \int_0^t \Phi_\alpha(t-t')A(x,t')dt'. \quad (10)$$

Here, the kernel $\Phi_\alpha(t)$ is equal in Laplace $t \to u$ space to $\Phi_\alpha(u)$. When $\alpha = 0$, it reduces to the usual memory kernel of the master equation for the CTRW [3,18,19].

We now consider a linear velocity field $v(x) = \omega x$ where ω is a constant. Then Eq. (4) becomes

$$A(k,u) = \Psi(u+\alpha)A_0(k) + \Psi(u+\alpha)\lambda(k)i^-(k+v_k,u), \quad (11)$$

where the symbol $v_k = \tau_a\omega k$. In the limit $\tau_a \to 0$, Eq. (11) gives

$$A(k,u) \simeq \Psi(u+\alpha)A_0(k) + \Psi(u+\alpha)\lambda(k) \times [i^-(k,u) + v_k {i^-}'_k(k,u)]. \quad (12)$$

Here, ${i^-}'_k(k,u)$ denotes the first partial derivative of $i^-(k,u)$ with respect to k. We substitute (9) into (12) and get

$$A(k,u) = \Psi(u+\alpha)A_0(k) + \psi(u+\alpha)\lambda(k) \times [A(k,u) + v_k A'_k(k,u)], \quad (13)$$

where $A'_k(k,u)$ is the first derivative of $A(k,u)$ for the variable k. This simplifies further to the generalized master equation in Fourier-Laplace space for the A particles in an $A \to B$ reaction under subdiffusion on a linear moving fluid,

$$[1-\psi(u+\alpha)\lambda(k)]A(k,u) = \Psi(u+\alpha)A_0(k) + \psi(u+\alpha)\lambda(k)v_k A'_k(k,u). \quad (14)$$

Note that if the reaction is not involved in the system and the initial condition is defined as $A_0(x) = \delta(x)$, then Eq. (14) recovers the master equation,

$$[1-\psi(u)\lambda(k)]A(k,u) = v_k\psi(u)\lambda(k)A'_k(k,u) + \Psi(u) \quad (15)$$

for the CTRW on linear moving fluids in a one-dimensional lattice obtained by Compte in Ref. [16].

There is another way to obtain the generalized master equation (15) where the balance condition (3) is replaced by [3]

$$\frac{\partial A(x,t)}{\partial t} = i^+(x,t) - i^-(x,t) - \alpha A(x,t), \quad (16)$$

where the losses include two parts: $i^-(x,t)$ due to the particles' departure from the site (loss flux) and $\alpha A(x,t)$ due to the conversion, and $i^+(x,t)$ is the gain flux which can be represented by the loss flux [19],

$$i^+(x,t) = \int_{-\infty}^{+\infty} i^-(x',t)\lambda[x-x'-\tau_a v(x')]dx'. \quad (17)$$

Transforming $(x,t) \to (k,u)$ of (16), one has

$$uA(k,u) - A_0(k) = \frac{\int i^-(k',u)\eta(k,u+\alpha;k-k')dk'}{\psi(u+\alpha)} - i^-(k,u) - \alpha A(k,u). \quad (18)$$

By using (7) and (18), we can also obtain the relation equation (9). Substitute Eq. (9) into Eq. (18) and assume $v(x) = \omega x$ in the limit $\tau_a \to 0$, and we find

$$uA(k,u) - A_0(k) \simeq [\lambda(k) - 1]\Phi_\alpha(u)A(k,u) + \lambda(k)v_k \times \Phi_\alpha(u)A'_k(k,u) - \alpha A(k,u). \quad (19)$$

Using $\Phi_\alpha(u) = \frac{(u+\alpha)\psi(u+\alpha)}{1-\psi(u+\alpha)}$ and $\Psi(u+\alpha) = \frac{1-\psi(u+\alpha)}{u+\alpha}$, one finally recovers the generalized master equation (14). This means that the two approaches to derive the generalized master equation for A particles in the reaction-subdiffusion process on moving fluids are equivalent. In what follows we will not distinguish them for A particles.

Inverting Eq. (19) to the space-time domain, we can obtain the master equation in the space-time domain,

$$\frac{\partial A(x,t)}{\partial t} + \tau_a \int_{-\infty}^{+\infty} dx' \int_0^t \Phi_\alpha(t-t')\lambda(x-x') \times \frac{\partial v(x')A(x',t')}{\partial x'} dt' = \int_{-\infty}^{+\infty} dx' \int_0^t \Phi_\alpha(t-t')[\lambda(x-x') - \delta(x-x')] \times A(x',t')dt' - \alpha A(x,t), \quad (20)$$

where the reaction rate explicitly affects both the diffusion term,

$$\int_{-\infty}^{+\infty} dx' \int_0^t \Phi_\alpha(t-t')[\lambda(x-x') - \delta(x-x')]A(x',t')dt',$$

and the advection term,

$$\tau_a \int_{-\infty}^{+\infty} dx' \int_0^t \Phi_\alpha(t-t')\lambda(x-x') \frac{\partial v(x')A(x',t')}{\partial x'} dt'.$$

Specifically, we consider a discrete random walk where the PDF of particles A on site $x = i$ at time t is denoted as $A(i,t)$, and the jump PDF is assumed to be $\lambda(-1) = \frac{1}{2}$, $\lambda(1) = \frac{1}{2}$, meaning that the particle can jump from $x = i$ to the adjacent grid point to the right and left directions with the same probability. If $v(x) = 0$, then Eq. (20) reduces to

$$\frac{\partial A(i,t)}{\partial t} = \int_0^t \Phi_\alpha(t-t')\left[\frac{1}{2}A(i-1,t) + \frac{1}{2}A(i+1,t) - A(i,t)\right]dt' - \alpha A(i,t) \quad (21)$$

obtained by Sokolov *et al.* in Ref. [3].

We now turn to apply the master equation (19) to derive an ADRE for Gaussian jump length $\lambda(k) \sim 1 - \frac{\sigma^2 k^2}{2}$ and long-tailed waiting time $\psi(u) \sim 1 - \Gamma(1-\beta)(\tau u)^\beta$ with σ^2 being the jump length variance and $0 < \beta < 1$ and τ, respectively, being the anomalous exponent and the appropriate timescale. Assuming $A_0(x) = \delta(x)$, substituting $\Phi_\alpha(u) = \frac{1}{\tau^\beta \Gamma(1-\beta)}(u+\alpha)^{1-\beta}$ [3] into the master equation (19) in the limit of $\tau \to 0$, $\sigma \to 0$, and $\tau_a \to 0$, we obtain

$$uA(k,u) - 1 \simeq -K_\beta k^2 (u+\alpha)^{1-\beta} A(k,u) + C_\beta (u+\alpha)^{1-\beta} \omega k A'_k(k,u) - \alpha A(k,u), \quad (22)$$

where the generalized diffusion coefficient $K_\beta = \lim_{\tau\to 0,\, \sigma \to 0} \frac{\sigma^2}{2\tau^\beta \Gamma(1-\beta)}$ and advection coefficient $C_\beta = \lim_{\tau_a \to 0,\, \tau \to 0} \frac{\tau_a}{\tau^\beta \Gamma(1-\beta)}$ are kept finite. Inverting Eq. (22) to the space-time domain $k \to x$ and $s \to t$, using the fact that $\mathcal{F}[xf(x)] = i\frac{\partial}{\partial k} f(k)$, we then get the generalized ADRE for the A particle in the reaction-subdiffusion process on linear flows,

$$\frac{\partial A(x,t)}{\partial t} + C_\beta e^{-\alpha t} {}_0D_t^{1-\beta}\left[e^{\alpha t} \frac{\partial [v(x)A(x,t)]}{\partial x}\right] = K_\beta e^{-\alpha t} {}_0D_t^{1-\beta}\left[e^{\alpha t} \frac{\partial^2 A(x,t)}{\partial x^2}\right] - \alpha A(x,t), \quad (23)$$

with the initial condition $A_0(x) = \delta(x)$. Here, the diffusion and advection operator [8,20],

$$e^{-\alpha t} {}_0D_t^{1-\beta}[e^{\alpha t} f(t)] = \frac{1}{\Gamma(\beta)}\left(\frac{d}{dt}\int_0^t \frac{e^{-\alpha(t-t')}}{(t-t')^{1-\beta}} f(t')dt' + \alpha \int_0^t \frac{e^{-\alpha(t-t')}}{(t-t')^{1-\beta}} f(t')dt'\right) \quad (24)$$

is reaction dependent, equal in Laplace $t \to u$ space to $(u+\alpha)^{1-\beta} f(u)$, and when $\alpha = 0$ it becomes ${}_0D_t^{1-\beta} f(t)$ which is the Riemann-Liouville fractional derivative operator [4,21]. Note that for a nonreactive system, Eq. (23) reduces to the classical fractional diffusion-advection equation [16,22]. Note also that, in the absence of an advection velocity field, i.e., $v(x) = 0$, we can recover the coupled fractional reaction-diffusion equation for species A with a two-species irreversible linear reaction under subdiffusion derived in Ref. [8].

In particular, in the presence of a constant drag velocity field, i.e., $v(x) = \frac{v^*}{C_\beta}$, Eq. (23) becomes

$$\frac{\partial A(x,t)}{\partial t} + v^* e^{-\alpha t} {}_0D_t^{1-\beta}\left[e^{\alpha t} \frac{\partial A(x,t)}{\partial x}\right] = K_\beta e^{-\alpha t} {}_0D_t^{1-\beta}\left[e^{\alpha t} \frac{\partial^2 A(x,t)}{\partial x^2}\right] - \alpha A(x,t) \quad (25)$$

with the initial condition $A_0(x) = \delta(x)$. Fourier transforming $x \to k$ and Laplace transforming $t \to u$ of Eq. (25) yields

$$A(k,u) = \frac{1}{u + \alpha + K_\beta k^2 (u+\alpha)^{1-\beta} + v^* i k (u+\alpha)^{1-\beta}}. \quad (26)$$

By using Eq. (26), the relation [23],

$$\langle x^n \rangle(u) = i^n \lim_{k\to 0} \frac{\partial^n A(k,u)}{\partial k^n}, \quad (27)$$

and the Laplace inversion, one obtains the moments of reaction-subdiffusion process for the A particles in Galilei variant velocity flows,

$$\langle x \rangle(t) = \frac{v^* t^\beta e^{-\alpha t}}{\Gamma(1+\beta)}, \quad (28)$$

$$\langle (\Delta x)^2 \rangle(t) = \frac{2K_\beta t^\beta e^{-\alpha t}}{\Gamma(1+\beta)} + (v^*)^2 t^{2\beta} \times \frac{2e^{-\alpha t}\Gamma^2(1+\beta) - e^{-2\alpha t}\Gamma(1+2\beta)}{\Gamma(1+2\beta)\Gamma^2(1+\beta)}. \quad (29)$$

Consequently, the first moment contains a sublinear growth due to subdiffusion and an exponential decay depending on the reaction rate with time, and the drag along the velocity field v^*. The first term of the mean squared displacement provides the reaction-subdiffusion process in the absence of velocity fields, and the second one describes the coupling between the reaction under subdiffusion and the drag velocity. When $\alpha = 0$, the above results (28) and (29) reduce to

$$\langle x\rangle(t) = \frac{v^* t^\beta}{\Gamma(1+\beta)}, \tag{30}$$

$$\langle(\Delta x)^2\rangle(t) = \frac{2K_\beta t^\beta}{\Gamma(1+\beta)} + (v^*)^2 t^{2\beta} \times \frac{2\Gamma^2(1+\beta) - \Gamma(1+2\beta)}{\Gamma(1+2\beta)\Gamma^2(1+\beta)}, \tag{31}$$

which are in agreement with the behaviors for the Galilei variant fractional diffusion-advection process in Ref. [22]. Note that Eqs. (30) and (31) are also the asymptotic forms of Eqs. (28) and (29) for short times when the effects of the reaction are too small to negligible.

We now make the substitution,

$$A(x,t) = e^{-\alpha t} W_\beta(x,t), \tag{32}$$

with A and W_β having the same initial condition. From Eq. (26) we find $W_\beta(x,t)$ is the inverse Fourier and Laplace transforms of expression,

$$W_\beta(k,u) = \frac{1}{u + K_\beta k^2 u^{1-\beta} + v^* iku^{1-\beta}}. \tag{33}$$

This propagator is led to the Galilei variant fractional diffusion-advection equation [4,22],

$$\frac{\partial W_\beta(x,t)}{\partial t} = {}_0D_t^{1-\beta}\left(-v^*\frac{\partial}{\partial x} + K_\beta \frac{\partial^2}{\partial x^2}\right) W_\beta(x,t), \tag{34}$$

whose normalized solution $W_\beta(x,t)$ can be expressed by the Brownian solution $W_1(x,t) = \frac{1}{\sqrt{4\pi t}}\exp\left(-\frac{(x-t)^2}{4t}\right)$ through an integral relation,

$$W_\beta(x,t) = \int_0^{+\infty} F(s,t) W_1(x,s) ds \tag{35}$$

for $v, K \equiv 1$, where the kernel $F(s,t)$ is represented in terms of a Fox function,

$$F(s,t) = \frac{1}{s\beta} H_{1,1}^{1,0}\left[\frac{s^{1/\beta}}{t}\middle|_{(1,1/\beta)}^{(1,1)}\right], \tag{36}$$

which reduces to $F(s,t) = (\pi t)^{-0.5} e^{-s^2/(4t)}$ for $\beta = 0.5$. Thus, the normalized solution of the generalized ADRE (23) for the A particle in the reaction-subdiffusion process in the Galilei variant moving flows is

$$A(x,t) = e^{-\alpha t} \int_0^{+\infty} F(s,t) W_1(x,s) ds, \tag{37}$$

which features a reactive effect $e^{-\alpha t}$. In Figs. 1 and 2 $A(x,t)$ and $W_\beta(x,t)$ are shown at various times in the case $\alpha = 0.15$. It should be noted that the solution $A(x,t)$ is asymmetric with respect to the maximum which stays fixed at the origin because of the effect of the convection velocity, and it decays with time to zero more rapidly than $W_\beta(x,t)$.

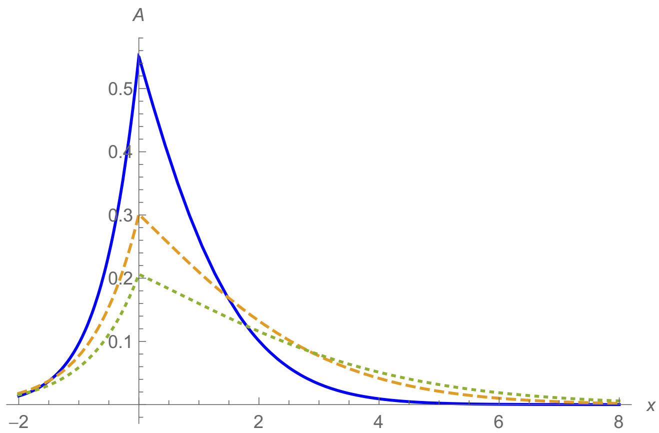

FIG. 1. The time evolution of the PDF for the A particle in the reaction-subdiffusion process in flows with reaction rate $\alpha = 0.15$ and anomalous diffusion exponent $\beta = 0.5$. The solution is shown for the dimensionless times $t = 0.2$ (solid line), 1 (dashed line), and 2 (dotted line). It is asymmetric with respect to the Y axis, and the plume stretches more and more into the direction of the convection velocity. Moreover, the decay with time is faster than that in nonreactive process in Fig. 2 because of the negative exponential decay accounting for the effect of the $A \to B$ reaction.

B. CTRW scheme for B particles and corresponding ADRE

Analogously we will now derive the generalized master equation for the B particles. Let $B(x,t)$ be the PDF of the 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 the 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 $t' > 0$ and still keeps at (or just leaves) site x at time t, we give the following balance

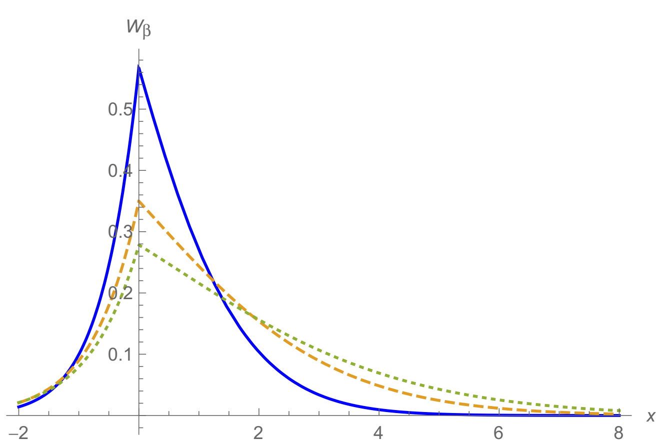

FIG. 2. The evolution of the PDF for the particle in the nonreactive Galilei variant subdiffusive model with reaction rate $\alpha = 0$ and mean flight time $\beta = 0.5$. The solution is shown for the dimensionless times $t = 0.2$ (solid line), 1 (dashed line), and 2 (dotted line). The propagator is asymmetric with respect to the maximum which stays fixed at the origin since the anomalous particle is dragged along with the drift velocity [4,22].

equations:

$$B(x,t)=\int_{-\infty}^{+\infty}dx'\int_0^t j^-(x',t')\phi(x-x',t-t';x')dt' + \int_{-\infty}^{+\infty}dx'\int_0^t i^-(x',t')\phi(x-x',t-t';x') \times(1-e^{-\alpha(t-t')})dt' + A_0(x)\Psi(t)(1-e^{-\alpha t}), \tag{38}$$

and

$$j^-(x,t)=\int_{-\infty}^{+\infty}dx'\int_0^t j^-(x',t')\eta(x-x',t-t';x')dt' + \int_{-\infty}^{+\infty}dx'\int_0^t i^-(x',t')\eta(x-x',t-t';x') \times(1-e^{-\alpha(t-t')})dt' + A_0(x)\psi(t)(1-e^{-\alpha t}), \tag{39}$$

where the initial condition $B(x,t)=0$ was used. Laplace $x\to k$ and Fourier $t\to u$ transforming of the two equations (25) and (26) yields

$$B(k,u)=\int j^-(k',u)\phi(k,u;k-k')dk' + \int i^-(k',u)[\phi(k,u;k-k') - \phi(k,u+\alpha;k-k')]dk' + [\Psi(u)-\Psi(u+\alpha)]A_0(k), \tag{40}$$

and

$$j^-(k,u)=\int j^-(k',u)\eta(k,u;k-k')dk' + \int i^-(k',u)[\eta(k,u;k-k') - \eta(k,u+\alpha;k-k')]dk' + [\psi(u)-\psi(u+\alpha)]A_0(k). \tag{41}$$

In the above expressions $B(k,u)$ and $j^-(k,u)$ represent the Fourier-Laplace transforms of $B(x,t)$ and $j^-(x,t)$, respectively. Comparing (4), (7), (40), and (41), one has

$$\frac{A(k,u)+B(k,u)}{\Psi(u)}=\frac{i^-(k,u)+j^-(k,u)}{\psi(u)}, \tag{42}$$

which can be changed to the form

$$j^-(k,u)=\Phi_0(u)B(k,u)+[\Phi_0(u)-\Phi_\alpha(u)]A(k,u). \tag{43}$$

When $v(x)=0$ it is consistent with the result obtained in Ref. [3].

If Eq. (38) is replaced by the balance equation,

$$\frac{\partial B(x,t)}{\partial t}=\int_{-\infty}^{+\infty} j^-(x',t)\lambda[x-x'-\tau_a v(x')]dx' - j^-(x,t)+\alpha A(x,t), \tag{44}$$

we can also find Eq. (43) by using (7), (18), and (41), the transform $(x,t)\to(k,u)$ of Eq. (44),

$$B(k,u)=\frac{\int j^-(k',u)\eta(k,u+\alpha;k-k')dk'}{\psi(u+\alpha)} - j^-(k,u)+\alpha A(k,u), \tag{45}$$

and the relation $\Psi(u)=\frac{1-\psi(u)}{u}$. It means that the two ways using different balance conditions for B particles are equivalent, too.

In linear flow $v(x)=\omega x$ Eq. (45) can be written in the form

$$B(k,u)\simeq\lambda(k)j^-(k+v_k,u)-j^-(k,u)+\alpha A(k,u) \tag{46}$$

for small τ_a. Substitution of (43) into Eq. (46) gives the master equation for the PDF of the B particle in Fourier-Laplace space,

$$uB(k,u)=\lambda(k)v_kB_k'(k,u)\Phi_0(u)+\lambda(k)v_kA_k'(k,u) \times[\Phi_0(u)-\Phi_\alpha(u)]+[\lambda(k)-1]B(k,u)\Phi_0(u) + [\lambda(k)-1]A(k,u)[\Phi_0(u)-\Phi_\alpha(u)]+\alpha A(k,u), \tag{47}$$

where ${B'}_k(k,u)$ is the partial derivative of $B(k,u)$ with respect to the variable k. Inverting the above equation to the space-time domain, we obtain the master equation in the space-time domain,

$$\frac{\partial B(x,t)}{\partial t}+\tau_a\int_{-\infty}^{+\infty}dx'\int_0^t\Phi_0(t-t')\lambda(x-x')\frac{\partial v(x')B(x',t')}{\partial x'}dt' + \tau_a\int_{-\infty}^{+\infty}dx'\int_0^t[\Phi_0(t-t')-\Phi_\alpha(t-t')]\lambda(x-x')\frac{\partial v(x')A(x',t')}{\partial x'}dt' = \int_{-\infty}^{+\infty}dx'\int_0^t[\Phi_0(t-t')-\Phi_\alpha(t-t')][\lambda(x-x')-\delta(x-x')]A(x',t')dt' + \int_{-\infty}^{+\infty}dx'\int_0^t\Phi_0(t-t')[\lambda(x-x')-\delta(x-x')]B(x',t')dt'+\alpha A(x,t). \tag{48}$$

Note that, in the master equation (48), the first and second terms on the right hand side which depend on the reaction rate α compose the diffusion part and the terms,

$$\tau_a \int_{-\infty}^{+\infty} dx' \int_0^t \Phi_0(t-t')\lambda(x-x')\frac{\partial v(x')B(x',t')}{\partial x'}dt',$$

and

$$\tau_a \int_{-\infty}^{+\infty} dx' \int_0^t [\Phi_0(t-t') - \Phi_\alpha(t-t')]\lambda(x-x') \times \frac{\partial v(x')A(x',t')}{\partial x'}dt',$$

on the left hand side of the equation represent the effects of the advection velocity fields. For a discrete random walk with $v(x) = 0$, the jump PDF satisfies $\lambda(-1) = \frac{1}{2}$, $\lambda(1) = \frac{1}{2}$, and in the continuum limit, Eq. (48) reduces to the result in Ref. [3]. If we substitute the Gaussian jump length $\lambda(k) \sim 1 - \frac{\sigma^2 k^2}{2}$ and power law waiting time PDF $\psi(u) \sim 1 - \Gamma(1-\beta)(\tau u)^\beta$ into the master equation (47) and invert $k \to x$, $u \to t$, in the limit of small τ_a, τ, and σ, we then find the generalized ADRE for the B particle in the reaction $A \to B$ under subdiffusion in the linear velocity field,

$$\frac{\partial B(x,t)}{\partial t} + C_\beta\, {}_0D_t^{1-\beta}\frac{\partial[v(x)B(x,t)]}{\partial x} + C_\beta\big[{}_0D_t^{1-\beta} - e^{-\alpha t}\,{}_0D_t^{1-\beta}(e^{\alpha t})\big]\frac{\partial[v(x)A(x,t)]}{\partial x} \simeq K_\beta\,{}_0D_t^{1-\beta}\frac{\partial^2 B(x,t)}{\partial x^2} + \alpha A(x,t) + K_\beta\big[{}_0D_t^{1-\beta} - e^{-\alpha t}\,{}_0D_t^{1-\beta}(e^{\alpha t})\big]\frac{\partial^2 A(x,t)}{\partial x^2}. \quad (49)$$

It should be noted that in (49) both advection and diffusion terms couple with the reaction since in these two terms the parameter of the reaction explicitly enters the diffusion and advection operators but also that there are the fractional kinetics memories at previous times for the A particle. Note also that Eq. (49) can reduce to the fractional reaction-diffusion equation for species B for the subdiffusive system with linear reaction $A \to B$ [8] when $v(x) = 0$. For a constant velocity $v(x) = \frac{v^*}{C_\beta}$, Eq. (49) becomes

$$\frac{\partial B(x,t)}{\partial t} + v^*\,{}_0D_t^{1-\beta}\frac{\partial B(x,t)}{\partial x} + v^*\big[{}_0D_t^{1-\beta} - e^{-\alpha t}\,{}_0D_t^{1-\beta}(e^{\alpha t})\big]\frac{\partial A(x,t)}{\partial x} \simeq K_\beta\,{}_0D_t^{1-\beta}\frac{\partial^2 B(x,t)}{\partial x^2} + \alpha A(x,t) + K_\beta\big[{}_0D_t^{1-\beta} - e^{-\alpha t}\,{}_0D_t^{1-\beta}(e^{\alpha t})\big]\frac{\partial^2 A(x,t)}{\partial x^2} \quad (50)$$

with the initial conditions $A_0(x) = \delta(x)$ and $B_0(x) = 0$. By transforming $(x,t) \to (k,u)$ of (50), using Eqs. (26), (27), and the Laplace inversion, we find the first two moments for the reaction-subdiffusion process of B particles in Galilei variant velocity flows,

$$\langle x\rangle(t) = \frac{v^* t^\beta}{\Gamma(1+\beta)}(1 - e^{-\alpha t}), \quad (51)$$

$$\langle(\Delta x)^2\rangle(t) = \frac{2K_\beta t^\beta}{\Gamma(1+\beta)}(1-e^{-\alpha t}) + (v^*)^2 t^{2\beta} \times \frac{2\Gamma^2(1+\beta)(1-e^{-\alpha t}) - \Gamma(1+2\beta)(1-e^{-2\alpha t})^2}{\Gamma(1+2\beta)\Gamma^2(1+\beta)}. \quad (52)$$

These results show the complex coupling relations between velocity field and chemical reaction under subdiffusion carry over to the moments for the B particle. It should be noted that the moments of the process shown in (51) and (52) contain the term $1 - e^{-\alpha t}$ which reflects the effect on the evolution for the B particle of the reaction $A \to B$ and differs from $e^{-\alpha t}$ including in the moments for the A particle. This interesting behavior is also found in the evolution of the PDF for the B particles as shown below. Combining (25) with (50), one has

$$\frac{\partial[A(x,t)+B(x,t)]}{\partial t} = {}_0D_t^{1-\beta}\left[-v^*\frac{\partial}{\partial x} + K_\beta\frac{\partial^2}{\partial x^2}\right][A(x,t)+B(x,t)], \quad (53)$$

which is equivalent to Eq. (34) for subdiffusion in a nonreactive liquid, this is expected since the simple reaction we discuss here does not change the amount of all particles in the system. We then find $A(x,t) + B(x,t) = W_\beta(x,t)$ from which one can easily calculate the evolution of the PDF for the B particle,

$$B(x,t) = (1 - e^{-\alpha t})\int_0^{+\infty} F(s,t)W_1(x,s)ds, \quad (54)$$

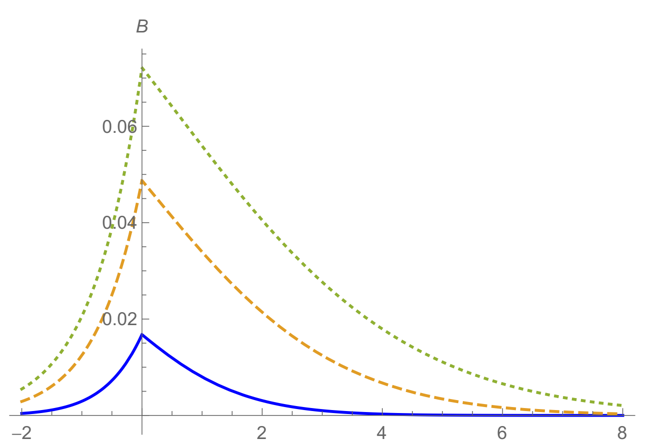

FIG. 3. The evolution of the PDF for the B particle in the reaction-subdiffusion process in flows with reaction rate $\alpha = 0.15$ and anomalous exponent $\beta = 0.5$. The solution is shown for the dimensionless times $t = 0.2$ (solid line), 1 (dashed line), and 2 (dotted line). The moving flows also result in the asymmetry of the solution for created particles with respect to the Y axis. The growth over time compares with the decay with time for $A(x,t)$ in Fig. 1.

which has the reactive characteristic $1 - e^{-\alpha t}$. As shown in Fig. 3, this asymmetric solution grows with time, exactly opposite to $A(x, t)$.

III. CONCLUSIONS

To sum up we derive the master equations (20) and (48) for the PDF of the A and B particles in a simple monomolecular conversion reaction $A \to B$ taking place at a constant rate α and under subdiffusion in linear flows. As examples, two generalized advection-diffusion reaction equations (23) and (49) are obtained, the first two moments and the solutions in Galilei variant constant velocity flows are also worked out, and the interesting couple relations among diffusion, advection, and reaction process are shown. There are problems, such as the dynamic behaviors for a more complex reaction under subdiffusion in moving fluids are still unknown.

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