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# Mesoscopic description of reactions for anomalous diffusion: a case study

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## Abstract

Reaction–diffusion equations deliver a versatile tool for the description of reactions in inhomogeneous systems under the assumption that the characteristic reaction scales and the scales of the inhomogeneities in the reactant concentrations separate. In the present work, we discuss the possibilities of a generalization of reaction–diffusion equations to the case of anomalous diffusion described in terms of continuous-time random walks with decoupled step length and waiting time probability densities, the first being Gaussian or Lévy, the second one being an exponential or a power law lacking the first moment. We consider a special case of an irreversible or reversible  $A \rightarrow B$  conversion and show that only in the Markovian case of an exponential waiting time distribution can the diffusion term and the reaction term be decoupled. In all other cases, the properties of the reaction affect the transport operator, so the form of the corresponding reaction–anomalous diffusion equations does not closely follow the form of the usual reaction–diffusion equations.

## 1. Introduction

Many phenomena in systems out of equilibrium can be described using a reaction–diffusion picture. Examples can be found in various disciplines, above all in chemistry but also in physics, ecology and others. Examples from physics include the trapping and annihilation of excitons and the electron–hole recombination in solids. In ecology, there are e.g. the predator–prey relations. Reaction–diffusion processes with both normal and anomalous diffusion have been extensively studied over the past decades. However, for the latter, a general theoretical framework is still absent. In this paper, we discuss a special case of monomolecular conversion for subdiffusion and show that the mesoscopic approach leads to equations different in form from what could be regarded as a straightforward generalization of the reaction–diffusion scheme.

The mesoscopic approach leading to reaction–diffusion equations is valid if there is a strong scale separation between the typical reaction scale and the size of the system’s inhomogeneities. The corresponding reaction–diffusion equations (for normal diffusion) typically have the form

$$\frac{\partial C_i(t)}{\partial t} = K_i \Delta C_i \pm \kappa_i C_1^{n_1} C_2^{n_2} \cdots C_N^{n_N}, \quad (1)$$

which simply follows by adding a diffusion term to a classical kinetic equation for the corresponding reaction. Here,  $K_i$  denotes the diffusivity of the component  $i$ , the integer powers  $n_j$  correspond to the stoichiometry of the reaction, and  $\kappa_i$  denotes the corresponding reaction rate.

However, many physical systems exhibit anomalous diffusion which is not adequately described by Fick’s law [1]. Many cases of subdiffusion are successfully modelled within the continuous-time random walk framework (CTRWs) with power-law on-site waiting time distributions lacking the first moment. These distributions typically have the form  $w(t) \propto t^{-1-\alpha}$  with  $0 < \alpha < 1$ . Examples include, among others, dispersive charge transport in disordered semiconductors, contaminant transport by underground water and motion of proteins through cell membranes. On the other hand, successful search strategies in animal motion can be described in terms of Lévy walks or flights, often in combination with broad waiting time distributions. Lévy flights are also used as a model for the transport on annealed polymer chains [2, 3], which may be relevant for gene expression [4].

For anomalous diffusion, the Fickian diffusion equation is changed for an anomalous diffusion equation involving fractional derivatives. For subdiffusion, the equation for the concentration  $C(x, t)$  of diffusing particles reads

$$\frac{\partial C(x, t)}{\partial t} = K_{\alpha 0} D_t^{1-\alpha} \Delta C(x, t), \quad (2)$$

with the corresponding (anomalous) diffusion coefficient  $K_{\alpha}$ , where  ${}_0 D_t^{\beta}$  stands for the operator of a fractional Riemann–Liouville derivative,

$${}_a D_x^{\beta} f(x) = \frac{d^n}{dx^n} \frac{1}{\Gamma(\nu)} \int_a^x \frac{f(x')}{(x-x')^{1-\nu}} dx' \quad (3)$$

with  $n = [\beta] + 1$  ( $[x]$  stands for the whole part of the number  $x$ ) and  $\nu = n - \beta$ . For a Lévy flight, i.e. the random walk process with the power-law distribution of the step lengths,  $\lambda(x) \propto x^{-1-\mu}$ , the corresponding equation reads

$$\frac{\partial C(x, t)}{\partial t} = K_{\mu} \Delta^{\mu/2} C(x, t), \quad (4)$$

where  $\Delta^{\mu/2}$  stands for the Riesz symmetric fractional derivative acting on the spatial variable [5]. For a ‘sufficiently well-behaved’ function  $f(x)$  it can be expressed through the Liouville–Weyl derivative [6]:

$$\Delta^{\mu/2} f(x) = -\frac{1}{2 \cos(\pi \mu)} [{}_{-\infty} D_x^{\mu} + {}_x D_{\infty}^{\mu}] \quad (5)$$

for  $\mu \neq 1/2$ , and for  $\mu = 1/2$  through the derivative of the Hilbert transform of  $f$ :

$$\Delta^{1/2} f(x) = -\frac{d}{dx} \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\phi(\xi) d\xi}{x - \xi}. \quad (6)$$

Reactions under anomalous diffusion were discussed by several authors. However, most attention was paid to the description of the elementary act of reaction on the microscopic

scale [7–11]. Mesoscopic approaches were used e.g. in [12] for subdiffusion, where equations of the type

$$\frac{\partial C_i(\mathbf{r}, t)}{\partial t} = K_{i,\alpha_i} D_t^{1-\alpha_i} \Delta C_i(\mathbf{r}, t) + f_i \quad (7)$$

were postulated for different components in a multi-component system, and in [13, 14], where front propagation was discussed for symmetric and asymmetric Lévy flights, respectively; see also [15] and [4], where a Lévy diffusion term was added to a ‘normal’ reaction–diffusion equation to describe target search processes on the DNA.

In what follows, we discuss the derivation of the reaction–anomalous diffusion equations for a special case of the simple monomolecular conversion  $A \rightarrow B$  for a CTRW transport mechanism (where our approach however differs from that of our previous publication [16]). We consider subdiffusion, Lévy flights and the combination of the two. Moreover, a reversible conversion  $A \rightleftharpoons B$  is also considered. As we proceed to show, the Markovian situation of a (symmetric) Lévy flight is described correctly by the reaction–superdiffusion equation

$$\frac{\partial C_i(\mathbf{r}, t)}{\partial t} = K_{\mu_i} \Delta^{\mu_i/2} C_i(\mathbf{r}, t) + f_i \quad (8)$$

with  $C_i$  being  $A$  or  $B$  and the reaction terms  $f_i = \pm \kappa A$ . On the other hand, the situation for the non-Markovian subdiffusive transport is much more involved. The irreversible reaction can be described by an equation for  $A$  with the transport term depending on the reaction rate, and the equation for the reversible case cannot be cast in the form of something resembling a reaction–diffusion equation.

The article is structured as follows. In section 2 we derive the equation for the time evolution of the educt concentration  $A$  in an irreversible reaction. The behaviour of the product concentration  $B$  is discussed in section 3. Section 4 is devoted to a mesoscopic approach to reversible conversions.

## 2. The educt concentration in the irreversible conversion $A \rightarrow B$

In what follows, we consider the situation where  $A$ -particles are converted into  $B$  at a constant conversion rate  $\kappa$  independent of their position. Thus, the survival probability of a single  $A$ -particle in the time interval  $[t', t]$  is  $\Phi_A(t, t') = \Phi_A(t - t') = \exp[-\kappa(t - t')]$ . We will use one-dimensional notation in the following; the generalization to higher dimensions is straightforward. An example for this situation is the decay of a radioactive isotope in groundwater, where the reaction and the transport mechanism are fully decoupled. We are interested in the mathematical description of the situation, where the transport is given by a decoupled CTRW process with given step length and waiting time distribution. Our derivation of reaction–anomalous diffusion equations is parallel to the derivation of the pure anomalous diffusion equations in [1].

We can put down an equation for the probability density function (pdf) of the positions  $x$  of the particles, which have just made a jump at time  $t$ :

$$\eta_A(x, t) = \int_{-\infty}^{\infty} \int_0^t \eta_A(x', t') e^{-\kappa(t-t')} \psi(x - x', t - t') dx' dt' + A(x, 0) \delta(t). \quad (9)$$

Here,  $\psi(x, t)$  is the jump pdf given by the probability density in space and time to make a jump of length  $x$  at time  $t$  after the last jump. The meaning of the equation is that for whatever  $t > 0$  an  $A$ -walker that has just arrived at  $x$  has come there from some other site, where it had survived as  $A$  during the whole waiting time. The second term corresponds to the initial condition that at time  $t = 0$  all particles are assigned a new waiting time. Here, we have additionally assumed

that the jump length distribution does not depend on the position of the walker and that the waiting time pdf is constant in time and space. Furthermore,  $\psi(x - x', t - t')$  is assumed to be decoupled  $\psi(x - x', t - t') = \lambda(x - x')w(t - t')$ .

In order to get the equation of motion for the  $A$ -particles, i.e. for the concentration  $A(x, t)$ , we connect it to  $\eta_A(x, t)$  over

$$A(x, t) = \int_0^t dt' \eta_A(x, t') e^{-\kappa(t-t')} \Psi(t - t'), \quad (10)$$

where  $\Psi(t - t')$  is the probability of staying at site  $x$  for a time  $(t - t')$  after a jump. It is given by

$$\Psi(t) = 1 - \int_0^t dt' w(t'). \quad (11)$$

Both equations (9) and (10) contain convolution integrals and can be solved with Fourier–Laplace transforms. Using the shift theorem for the Laplace transform, we get

$$\hat{A}(k, u) = \frac{[1 - \tilde{w}(u + \kappa)] \hat{A}(k, 0)}{(u + \kappa)[1 - \hat{\psi}(k, u + \kappa)]}. \quad (12)$$

Before we can return to the space and time domain, we have to specify the jump pdfs. We are interested in the continuum limit of the equations corresponding to large scales and long times, i.e. to  $(k, u) \rightarrow (0, 0)$ . A characteristic function of a Gaussian jump length pdf with variance  $2\sigma^2$  will then be approximated by  $\hat{\lambda}(k) \simeq 1 - k^2\sigma^2$ . A characteristic function of a broad Lévy distribution,  $\hat{\lambda}(k) = \exp(-\sigma^\mu |k|^\mu)$ , can be approximated through  $\hat{\lambda}(k) \simeq 1 - \sigma^\mu |k|^\mu$ . For a broad waiting time pdf of a Pareto (power-law) type,  $w(t) \simeq \alpha \tau^\alpha t^{-1-\alpha}$ , one infers the following asymptotics in Laplace space using a Tauberian theorem,  $\tilde{w}(u) \simeq 1 - \Gamma(1 - \alpha) u^\alpha \tau^\alpha$ . For the Markovian case, as exemplified by the exponential waiting time pdf,  $w(t) = \tau^{-1} \exp(-t/\tau)$ , one has  $\tilde{w}(u) \simeq 1 - u\tau$  in the continuum limit, which corresponds to  $\alpha = 1$ . Equation (12) then can be rewritten in the following form:

$$u \hat{A}(k, u) - \hat{A}(k, 0) = -(u + \kappa)^{1-\alpha} \frac{\sigma^\mu}{\Gamma(1 - \alpha) \tau^\alpha} |k|^\mu \hat{A}(k, u) - \kappa \hat{A}(k, u) \quad (13)$$

simplifying the inverse transforms. For the inverse Fourier transformation, we use  $\mathcal{F}^{-1}\{-k^2 \hat{f}(k)\} = \Delta f(x)$ , and  $\mathcal{F}^{-1}\{-|k|^\mu \hat{f}(k)\} = \Delta^{\mu/2} f(x)$ . Moreover, we introduce the notation  $K_{\mu, \alpha} = \sigma^\mu [\tau^\alpha \Gamma(1 - \alpha)]^{-1}$  for what later will be identified as the generalized diffusion coefficient. The inverse Laplace transform of the left-hand side of the equation is simply the first time derivative, since  $\mathcal{L}^{-1}\{u \hat{g}(u) - g(0)\} = dg(t)/dt$ .

We first combine the Gaussian and Lévy distributed jump length pdf with an exponential waiting time pdf. In this case, the pre-factor of  $\hat{A}(k, u)$  in the first term on the right of the equation does not depend on  $u$ . After inverse transforming the equation, it becomes a time-independent operator acting on the concentration as a function of the coordinates. For a Gaussian jump length distribution, our equation (13) now reads

$$\frac{\partial A(x, t)}{\partial t} = K_{2,1} \Delta A(x, t) - \kappa A(x, t), \quad (14)$$

and for Lévy flights,

$$\frac{\partial A(x, t)}{\partial t} = K_{\mu,1} \Delta^{\mu/2} A(x, t) - \kappa A(x, t). \quad (15)$$

Hence, the separation of the transport term and the reaction term is perfectly exact. For Lévy flights, the Laplace operator is just changed for the Riesz–Weyl fractional derivative.

Now, we turn to subdiffusion and consider a Gaussian distribution of the step lengths ( $\mu = 2$ ) combined with a broad waiting time pdf of a Pareto type with  $0 < \alpha < 1$ . From equation (13) we then get

$$\frac{\partial A(x, t)}{\partial t} = K_{2,\alpha} \mathcal{T}_t(1 - \alpha, \kappa) \Delta A(x, t) - \kappa A(x, t), \quad (16)$$

with the transport operator  $\mathcal{T}_t(1 - \alpha, \kappa) \Delta$ , which is now time dependent,

$$\mathcal{T}_t(1 - \alpha, \kappa) f(t) = \frac{1}{\Gamma(\alpha)} \left( \frac{d}{dt} \int_0^t \frac{e^{-\kappa(t-t')}}{(t-t')^{1-\alpha}} f(t') dt' + \kappa \int_0^t \frac{e^{-\kappa(t-t')}}{(t-t')^{1-\alpha}} f(t') dt' \right). \quad (17)$$

Its form follows from the shift theorem for the Laplace transform. We see that the reaction parameter enters the transport term, and the transport operator  $\mathcal{T}_t(1 - \alpha, \kappa)$  reduces to a fractional derivative only for  $\kappa = 0$ . Using the Laplace transform property of the Riemann–Liouville fractional derivative,  $\mathcal{L}^{-1}\{u^{-\alpha} \hat{f}(u)\} = {}_0D_t^{-\alpha} f(t)$  for  $\alpha > 0$ , and using the shift theorem, the temporal part of a transport operator (in its action on the arbitrary function of time  $f(t)$ ) can be transformed into a form [17]

$$\mathcal{T}_t(1 - \alpha, \kappa) f(t) = \exp(-\kappa t) {}_0D_t^{1-\alpha} \{\exp(\kappa t) f(t)\}. \quad (18)$$

One can also easily formulate the equations for the combination of Pareto waiting times and Lévy jumps being of the form

$$\frac{\partial A(x, t)}{\partial t} = K_{\mu,\alpha} \mathcal{T}_t(1 - \alpha, \kappa) \Delta^{\mu/2} A(x, t) - \kappa A(x, t), \quad (19)$$

with  $\Delta^{\mu/2}$  denoting the symmetrized (Riesz–Weyl) spatial fractional derivative.

By the way, as shown in [18], an external force field can be included in the model over an asymmetric jump length distribution leading to a fractional Fokker–Planck equation with the time fractional operator changed for our operator  $\mathcal{T}_t(1 - \alpha, \kappa)$  and with an additional reaction term.

### 3. Equations for the product concentration

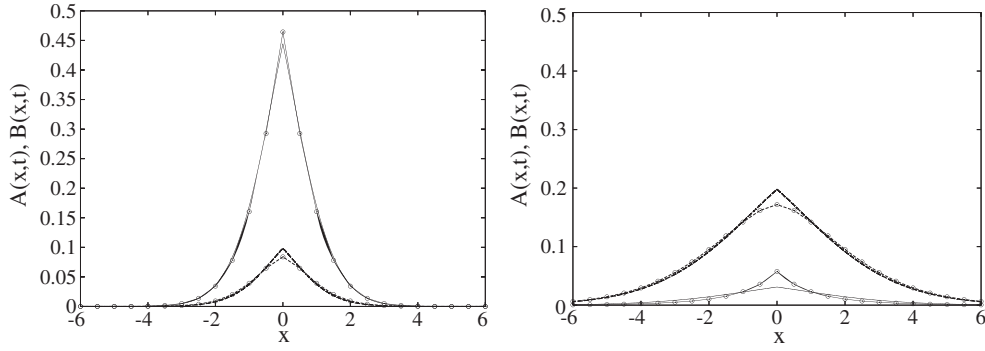
Let us turn to the equation for the concentration of the  $B$ -particles. One can distinguish two different cases: (i) either a  $B$ -particle takes over the waiting time of the  $A$ -particle that it was converted from; or (ii) we assign it a new waiting time when it is produced. The former means that the conversion is just a relabelling from the standpoint of diffusion and that conversion and transport are totally independent. The latter is appropriate when  $A$ - and  $B$ -particles have different diffusive properties, e.g. when they are trapped by different kinds of molecules. Then, transport and conversion are partly coupled.

(i) The first case corresponds to the following approach:

$$\eta_B(x, t) = \int_{-\infty}^{\infty} dx' \int_0^t dt' \left\{ \left[ \eta_B(x', t') + \eta_A(x', t') \left( 1 - e^{-\kappa(t-t')} \right) \right] \times \psi(x - x', t - t') \right\} + B(x, 0) \delta(t), \quad (20)$$

which expresses the fact that a  $B$ -particle that has just landed at  $x$  at time  $t$  has come from a site  $x'$  at prior time  $t'$ , where it had either come already as a  $B$ -particle or where it had been converted from an  $A$ -particle. For the concentration of  $B$ -particles, we have

$$B(x, t) = \int_0^t dt' \left[ \eta_B(x, t') + \eta_A(x, t') \left( 1 - e^{-\kappa(t-t')} \right) \right] \Psi(t - t'), \quad (21)$$



**Figure 1.** Shown are the concentrations of  $A$ -particles (solid lines) and  $B$ -particles (dashed lines) for subdiffusion with conversion. The correct results (solution of equations (16) and (23)) are shown without dots. They are compared to the solutions of the decoupled equations (7) shown with dots. The parameters are:  $\alpha = 0.75$ ,  $\kappa = 0.001$ ,  $K_\alpha^2 \simeq 7.76 \times 10^{-3}$ . The times shown are  $t = 200$  (left) and  $t = 2000$  (right).

with  $\Psi(t)$  from equation (11). Now, a  $B$ -particle that is at site  $x$  at time  $t$  has come there at a prior time  $t'$  either already as a  $B$ -particle or as an  $A$ -particle and has been converted in  $(t - t')$ . Equation (21) can also be solved with Fourier–Laplace transforms and equations (9), (16) and (20). First, we get

$$\hat{B}(k, u) + \hat{A}(k, u) = \frac{\hat{B}(k, 0) + \hat{A}(k, 0) \frac{1 - \tilde{w}(u)}{u}}{1 - \hat{\psi}(k, u)}, \quad (22)$$

which is essentially the Fourier–Laplace transformed subdiffusion equation for the sum of the concentrations  $C(x, t) = A(x, t) + B(x, t)$ . This is due to the fact that we have assumed a complete independence of the transport and the conversion and can already be seen on adding the two approaches of equations (9) and (20). Using the corresponding solutions for the concentration of  $A$ -particles, for a Poissonian waiting time pdf, one infers an equation of the form (1) or (8). For a power-law waiting time pdf and the initial conditions  $A(x, 0) = \delta(x)$ ,  $B(x) = 0$  we get

$$\begin{aligned} \frac{\partial B(x, t)}{\partial t} &= K_{2,\alpha} {}_0D_t^{1-\alpha} \Delta B(x, t) + \kappa A(x, t) \\ &+ K_{2,\alpha} [{}_0D_t^{1-\alpha} - \mathcal{T}_t(1 - \alpha, \kappa)] \Delta A(x, t). \end{aligned} \quad (23)$$

The change of the concentration of the  $B$ -particles depends on the concentration of the  $A$ -particles at all previous times. This is due to the fact that the  $B$ -particles are already ‘aged’ when produced and have a memory for the last jump they have made as an  $A$ -particle because of the non-Markovian nature of the waiting time pdf. As mentioned above, the combination with a Lévy distributed jump length pdf leads to the same result as equation (23) with the Laplace operator just changed for its fractional generalization.

In figure 1 we compare the correct solutions, i.e. the solutions of equations (16) and (23), with the solutions of the special cases of equation (7) for the conversion. We note an even qualitative difference, so the latter justified only by analogy to the normal diffusion case cannot be used as an approximation of the exact equations. In order to get these results, we did not actually have to solve equations (16) and (23) because we could specify the solution from the fact that  $C(x, t)$ , the sum of the concentrations of  $A$ - and  $B$ -particles, fulfils a pure subdiffusion equation. For the conversion reaction with the reaction independent of

the transport, the concentrations are just given by  $A(x, t) = C(x, t) \exp(-\kappa t)$ ,  $B(x, t) = C(x, t)[1 - \exp(-\kappa t)]$ , namely by the product of the overall particle concentration and the survival probability or the conversion probability, respectively. The solution of the pure subdiffusion equation for  $C(x, t)$  and the initial condition,  $C(x, 0) = \delta(x)$  is known. It is Fox's  $H$ -function:

$$C(x, t) = \frac{1}{4K_{2,\alpha}t^\alpha} H_{1,1}^{1,0} \left[ \frac{|x|}{\sqrt{K_{2,\alpha}t^\alpha}} \middle| \begin{matrix} (1 - \alpha/2, \alpha/2) \\ (0, 1) \end{matrix} \right]. \quad (24)$$

Fox's  $H$ -function can be calculated using a series expansion [1]. The equations of the form equation (7) were solved using a modification of a numerical scheme presented recently by Yuste *et al* [19]. The scheme is a combination of a forward-time-centred-space discretization and the Grünwald–Letnikov form of the fractional derivative.

- (ii) Let us now consider the second case and assume that  $B$ -particles are assigned a new waiting time at production. Here, we expect to get a decoupled equation of the form (7) because the past as an  $A$ -particle is 'forgotten'. We have to start from

$$\eta_B(x, t) = \int_{-\infty}^{\infty} \int_0^t \eta_B(x', t') \psi(x - x', t - t') dx' dt' + \kappa A(x, t) + B(x, 0)\delta(t), \quad (25)$$

and

$$B(x, t) = \int_0^{\infty} \eta_B(x, t') \Psi(t - t') dt'. \quad (26)$$

This leads first to

$$\hat{B}(k, u) = \frac{1 - \tilde{w}(u) \kappa \hat{A}(k, u) + \hat{B}(k, 0)}{u (1 - \hat{\psi}(k, u))}, \quad (27)$$

and then with a Gaussian jump length pdf and the same initial conditions as above to

$$\frac{\partial B(x, t)}{\partial t} = K_{2,\alpha_B} D_t^{1-\alpha_B} \Delta B(x, t) + \kappa A(x, t), \quad (28)$$

the expected decoupled equation. We have denoted the diffusion exponent as  $\alpha_B$  in order to emphasize that it is possibly different from that for the  $A$ -particles. By the way, instead of the reaction term  $\kappa A$  of the conversion we could have an arbitrary reaction term that does not depend on the product concentration.

#### 4. Reversible $A \rightleftharpoons B$ reaction

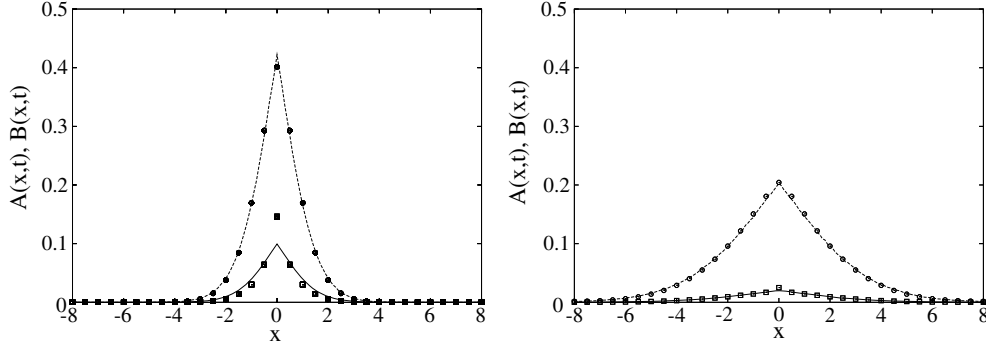
Now, we turn to the case of a reversible conversion. We assume that no new waiting time is assigned when a particle is converted. We denote the forward reaction rate by  $\kappa_1$  and the backward rate by  $\kappa_2$ . Then we have to start from

$$\eta_A(x, t) = \int_{-\infty}^{\infty} \int_0^t \left\{ \left[ \eta_A(x', t') e^{-\kappa_1(t-t')} + \eta_B(x', t') \left( 1 - e^{-\kappa_2(t-t')} \right) \right] \times \psi(x - x', t - t') dx' dt' \right\} + A(x, 0)\delta(t). \quad (29)$$

An  $A$ -walker that arrives at  $x$  at time  $t$  has come from another site  $x'$  at a prior time  $t'$ , where it had come already as an  $A$ -particle and was not converted, or where it had come as a  $B$ -particle and was converted. For the concentration, we have

$$A(x, t) = \int_0^t dt' \eta_A(x, t') e^{-\kappa_1(t-t')} \Psi(t - t') + \int_0^t dt' \eta_B(x, t') \left( 1 - e^{-\kappa_2(t-t')} \right) \Psi(t - t'). \quad (30)$$





**Figure 2.** Shown is the result of the simulation: *A*-particles (solid line) and *B*-particles (dashed line), and the numerical solution of the decoupled equations, equation (7) or (32): *A*-particles (squares) and *B*-particles (dots). The parameters are:  $\alpha = 0.75$ ,  $K_\alpha = 0.0138$ ,  $\kappa_1 = 0.01$ ,  $\kappa_2 = 0.001$ . The times shown are  $t = 200$  (left) and  $t = 2000$  (right).

An *A*-particle at site  $x$  at time  $t$  has come to this site already as an *A* at time  $t'$  and has not been converted and moved since, or it has come there as a *B*-particle, was converted and has not moved in the meantime. Because of the ‘symmetry’ of the reaction, the equations for the *B*-particles can be directly inferred from the equations for the *A*-particles. We can still perform Fourier–Laplace transformation. Using a Gaussian jump length pdf, an inverse power-law waiting time pdf, and the initial conditions  $A(x, 0) = \delta(x)$ ,  $B(x, 0) = 0$ , we find for the *A*-particles

$$\hat{A}(u, k) = \frac{K_{2,\alpha}k^2 + [(u + \kappa_1) - (u + \kappa_1)^{1-\alpha}u^\alpha] \times \dots}{[K_{2,\alpha}k^2 + (u + \kappa_2)^\alpha][K_{2,\alpha}k^2(u + \kappa_1)^{1-\alpha} + (u + \kappa_1)] + \dots} \times \frac{[u^{\alpha-1} - (u + \kappa_2)^{\alpha-1}] + (u + \kappa_2)^\alpha}{[u^\alpha(u + \kappa_1)^{1-\alpha} - (u + \kappa_1)][(u + \kappa_2)^\alpha - u^\alpha]} \quad (31)$$

However, after the inverse Fourier–Laplace transformation, the equation of motion does not take any simple form, let alone the form of a reaction–diffusion equation. The decoupled scheme, equation (7), corresponds to a different equation,

$$\hat{A}(u, k) = \frac{K_{2,\alpha}k^2 + \kappa_2u^{\alpha-1} + u^\alpha}{[K_{2,\alpha}k^2 + u^\alpha][K_{2,\alpha}k^2u^{1-\alpha} + u + \kappa_1 + \kappa_2]} \quad (32)$$

We have made some simple simulations in order to test how the decoupled equations perform for this case. For the conversion, the random walkers are independent, and we can simply repeat the random walk procedure many times ( $10^6$  times). We used the power-law waiting time pdf with a cut-off at small times guaranteeing the normalization,  $w(t) = \alpha\tau^\alpha t^{-1-\alpha}$  for  $t > \tau$  and  $w(t) = 0$  otherwise. The conversion is independent of the jumps and takes place with a constant probability  $P_{A,(B)} = [1 - \exp(-\kappa_{1,(2)}\Delta t)]$  in each time step of length  $\Delta t$ . We can see in figure 2 that the coincidence with the correct result is somewhat better for large times than in the case of an irreversible conversion.

## 5. Conclusions

We discussed generalizations of the reaction–diffusion scheme to the case of anomalous diffusion for a special case of a simple conversion reaction  $A \rightarrow B$  or  $A \rightleftharpoons B$ . Although the reaction and the particle transport were assumed to be independent, the reaction term and the

transport term do not separate in the case of subdiffusion. This means that the transport operator in the corresponding equations depends on the properties of the reaction. The simple equations with separated reaction and diffusion terms are not exact. Comparing the exact solution with the equations with decoupled reaction and diffusion terms shows that the latter deliver a rather poor approximation for the case of an irreversible reaction and perform somewhat better in the reversible case.

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