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Front propagation in reaction-dispersal with anomalous distributions

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Abstract. The speed of pulled fronts for parabolic fractional-reaction-dispersal equations is derived and analyzed. From the continuous-time random walk theory we derive these equations by considering long-tailed distributions for waiting times and dispersal distances. For both cases we obtain the corresponding Hamilton-Jacobi equation and show that the selected front speed obeys the minimum action principle. We impose physical restrictions on the speeds and obtain the corresponding conditions between a dimensionless number and the fractional indexes.

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1 Introduction

Fractional diffusion has been extensively presented as a useful approach for the description of transport dynamics in complex systems [1]. When fractional diffusion couples to reaction process wave fronts may exist. In such cases the number of particles or individuals grow at the same time that jump. Recently, some works have dealt with this topic. For anomalous waiting-time distributions the speed of fronts have been derived [2] and the conditions for the existence of diffusion-driven instability has been also studied [3]. For Lévy flights distributions, a fractional reaction-diffusion equation shows the existence of asymmetric fronts [4], that is, an accelerated front propagating to the right and a front propagating to the left with uniform speed.

In this work we present the mesoscopic Continuous-Time Random Walk (CTRW) as a phenomenological model to obtain temporal and spatial fractional reaction-diffusion equations. By calculating the Hamilton-Jacobi equation for each model we compute the front speed. Some of our results have been already published but we present them here as obtained from a single model in a simple and natural way. In particular, we obtain first a reaction-diffusion equation with a temporal fractional derivative by considering a fractal waiting-time probability distribution function (PDF) and classical spatial diffusion. This equation was previously obtained in [3], and its corresponding front speed in [2]. Secondly, we assume a classical (exponential) waiting-time PDF and a symmetric Lévy flight PDF to get a reaction-diffusion equation with a spatial fractional derivative. In [4], this equation was considered ad hoc, and its front speed obtained. Finally, we notice that those front speeds present an unphysical behaviour when the reaction-diffusion dimensionless number (the quotient between the characteristics waiting and reaction times) is sufficiently large. This constitutes the main result of this work.

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2 Anomalous reaction-dispersal equations

We derive first fractional reaction-dispersal equations (FRD) according by using the CTRW theory and considering the reaction process in a phenomenological way. The quantity which defines the motion is the probability distribution $\Psi(x,t)$ of the particle performing a jump of length x after waiting a time t at its starting point. If $P(x,t)$ is the number density of particles arriving at point x at time t and $\rho(x,t)$ is the number density of particles being at point x at time t, we have

$$P(x,t) = \int_{\mathbb{R}} dx' \int_0^t dt' \Psi(x-x',t-t')P(x',t') + P(x,t=0)\delta(t) + g(x,t) \quad (1)$$

$$\rho(x,t) = \int_0^t dt' \phi(t-t')P(x,t') \quad (2)$$

where $\phi(t)$ is the probability of remaining at least a time t on the point before proceeding with another jump, $P(x,t=0)$ is the initial distribution of particles and $g(x,t)$ is the number density of new particles created or generated at point x at time $t>0$. If $\varphi(t) = \int dx \Psi(x,t)$

is defined as the waiting time PDF, by the definition of $\phi(t)$ one has

$$\phi(t) = \int_t^\infty dt' \varphi(t'). \qquad (3)$$

The Fourier-Laplace transform of (2) is

$$P(k,s) = \Psi(k,s)P(k,s) + P(k,0) + g(k,s)$$
$$\rho(k,s) = P(k,s)\phi(s)$$

so that

$$\rho(k,s) = \frac{1-\varphi(s)}{s}\frac{f(k,s)}{1-\Psi(k,s)} \qquad (4)$$

where $f(k,s) \equiv P(k,0) + g(k,s)$ is the number density of new particles generated at time $t \geq 0$ and $s\phi(s) = 1 - \varphi(s)$ according to the Laplace transform of (3).

If the jump length and waiting time are independent random variables one finds the decoupled form $\Psi(x,t) = \Phi(x)\varphi(t)$ where $\Phi(x) = \int_0^\infty dt \Psi(x,t)$ is the jump length PDF. Inverting (4) by Fourier-Laplace we get a closed form for (2)

$$\rho(x,t) = \int_0^t dt' \varphi(t') \int_{\mathbb{R}} dx' \Phi(x')\rho(x-x', t-t') + \int_0^t dt' \phi(t') f(x, t-t'). \qquad (5)$$

In reaction-diffusion the local growth function f depends explicitly on ρ as a nonlinear function and we will consider that it is of the F-KPP (Fisher-Kolmogorov-Petrovskii-Piskunov) type [5,6] $f = r\rho(1-\rho)$ where r is the constant growth rate.

We consider now the specific waiting times PDF widely employed in fractional diffusion [1] in the Laplace space

$$\varphi(s) = e^{-(s\tau)^\gamma} \simeq 1 - (s\tau)^\gamma, \text{ for } 0 < \gamma \leq 1 \qquad (6)$$

for $t \gg \tau$ and the gaussian jump length PDF

$$\Phi(k) = e^{-\sigma^2 k^2} \simeq 1 - \sigma^2 k^2 \qquad (7)$$

for $|x| \gg \sigma$. The PDF in (6) is equivalent to a long-tailed waiting-time PDF with the asymptotic behavior $\varphi(t) \sim (\tau/t)^{1+\gamma}$ and may be considered as a generalization of $\varphi(s) = e^{-s\tau}$ corresponding to the case where there exists only an unique waiting time τ, that is $\varphi(t) = \delta(t-\tau)$.

Introducing (6) and (7) into (4) one has

$$\left[s + \sigma^2 k^2 s (s\tau)^{-\gamma}\right]\rho(k,s) = f(k,s)$$

which could be obtained also taking $\varphi(s) = [1 + (s\tau)^\gamma]^{-1}$ exactly. Inverting by Fourier-Laplace and using [1]

$$\mathcal{L}\left[{}_0\mathcal{D}_t^{1-\gamma}\rho(x,t)\right] = s^{1-\gamma}\rho(x,s)$$

one obtains

$$\partial_t \rho = \frac{\sigma^2}{\tau^\gamma}\ {}_0\mathcal{D}_t^{1-\gamma}\left(\partial_x^2 \rho\right) + f(\rho) \qquad (8)$$

where the Riemann-Liouville fractional derivative is defined by [1,8]

$${}_0\mathcal{D}_t^{1-\gamma}\rho(x,t) = \frac{1}{\Gamma(\gamma)}\partial_t \int_0^t dt' \frac{\rho(x,t')}{(t-t')^{1-\gamma}}, \text{ for } 0 < \gamma \leq 1. \qquad (9)$$

When reaction is absent ($f = 0$) then (8) describes a subdiffusive transport with $\langle x^2 \rangle \sim t^\gamma$.

Let us to consider now the classical waiting time PDF $\varphi(t) = \delta(t-\tau)$ with $t \gg \tau$ and a jump PDF describing symmetric Lévy flights with $\Phi(x) \sim \sigma^{2\alpha}|x|^{-1-2\alpha}$ for $|x| \gg \sigma$. Inserting

$$\varphi(s) = e^{-s\tau} \simeq 1 - s\tau \qquad (10)$$

$$\Phi(k) = e^{-(\sigma|k|)^{2\alpha}} \simeq 1 - (\sigma|k|)^{2\alpha} \text{ for } \frac{1}{2} \leq \alpha \leq 1 \qquad (11)$$

into (4) one has

$$\left[s\tau + \sigma^{2\alpha}|k|^{2\alpha}\right]\rho(k,s) = \tau f(k,s)$$

which may be inverted by Fourier-Laplace to yield the fractional reaction-Lévy equation

$$\partial_t \rho = \frac{\sigma^{2\alpha}}{\tau}\nabla^{2\alpha}\rho + f(\rho) \qquad (12)$$

where $\mathcal{F}\left[\nabla^{2\alpha}\rho(x,s)\right] = -|k|^{2\alpha}\rho(k,s)$ and the Riesz operator $\nabla^{2\alpha}$ reads [7,8]

$$\nabla^{2\alpha}\rho(x,t) = \frac{d^{2\alpha}\rho(x,t)}{d|x|^{2\alpha}} = -\frac{1}{2\cos(\alpha\pi)}\left(I_+^{-2\alpha} + I_-^{-2\alpha}\right) \qquad (13)$$

where

$$I_+^{2\alpha}\rho(x,t) = \frac{1}{\Gamma(2\alpha)}\int_{-\infty}^x (x-y)^{2\alpha-1}\rho(y,t)dy$$
$$I_-^{2\alpha}\rho(x,t) = \frac{1}{\Gamma(2\alpha)}\int_x^{+\infty} (y-x)^{2\alpha-1}\rho(y,t)dy$$

for $0 < \alpha \leq 1$.

Note that in absence of reaction, equation (12) describes a superdiffusive transport where the pseudo mean squared displacement [1] is $\left[x^2\right] \sim t^{1/\alpha}$ at large times (the mean squared displacement in the strict sense is divergent for the Lévy distribution).

3 Speed of fronts

Let us now illustrate how the speed of fronts may be derived for the fractional reaction-dispersal equation (8). As the growth function f is of F-KPP type the method we employ here has to allow us to obtain the linear speed selected by the front. We use the Hamilton-Jacobi formalism [6] but it is equivalent to use the marginal stability analysis. The starting point is the hyperbolic scaling

$x \to x/\varepsilon$ and $t \to t/\varepsilon$ and the redefinition of the field $\rho^\varepsilon(x,t) = \rho(x/\varepsilon, t/\varepsilon)$. Thus, equation (5) takes the form

$$\rho^\varepsilon(x,t) = \int_0^{t/\varepsilon} dt' \varphi(t') \int_{\mathbb{R}} dx' \Phi(x') \rho^\varepsilon(x - \varepsilon x', t - \varepsilon t') + \int_0^{t/\varepsilon} dt' \phi(t') \rho^\varepsilon(x, t - \varepsilon t') \left[1 - \rho^\varepsilon(x, t - \varepsilon t')\right]. \tag{14}$$

The rescaled number density of particles is, in the WKB form

$$\rho^\varepsilon(x,t) = \exp\left(-\frac{G^\varepsilon(x,t)}{\varepsilon}\right),\ G^\varepsilon(x,t) \geq 0, \tag{15}$$

where the action functional $G^\varepsilon(x,t)$ has to be found. From (15) as long as $G(x,t) = \lim_{\varepsilon\to 0} G^\varepsilon(x,t)$ is positive then $\rho^\varepsilon(x,t) \to 0$ as $\varepsilon \to 0$. The boundary of the set where $G^\varepsilon(x,t) > 0$ yields the position of the front. To ensure an evolution with the minimal propagation speed we take the initial condition $\rho(x,0) = 1$ for $x \leq 0$ and 0 for $x > 0$. Substitution of equation (15) into equation (14) and taking the limit $\varepsilon \to 0$ one gets the Hamilton-Jacobi equation [2]

$$\varphi^{-1}(H\tau) - \Phi(p) = \frac{a}{H\tau}\left[\varphi^{-1}(H\tau) - 1\right] \tag{16}$$

where

$$\varphi(H\tau) \equiv \int_0^\infty dt \varphi(t) e^{-Ht} = \varphi(s = H)$$
$$\Phi(p) \equiv \int_{-\infty}^\infty dx \Phi(x) e^{px} = \Phi(k = -ip) \tag{17}$$

and have defined the Hamiltonian $H = -\partial_t G$ and the generalized momentum $p = \partial_x G$. Finally, the front speed is computed from three equations: equation (16) and

$$v = \frac{\partial H}{\partial p},\ pv = H(p). \tag{18}$$

It is important to stress that the Hamilton-Jacobi equation (16) is equivalent to the dispersal relation if the speed was obtained from the marginal stability analysis.

4 Speed of temporal FRD fronts

In this section we compute the speed of fronts emerging from equation (8). From equations (17) and (6, 7) one obtains $\varphi^{-1}(H\tau) \simeq 1 + (H\tau)^\gamma$ and $\Phi(p) \simeq 1 + \sigma^2 p^2$ and inserting them into (16) one has

$$H^\gamma - rH^{\gamma-1} = \frac{\sigma^2}{\tau^\gamma} p^2. \tag{19}$$

Taking the derivative ∂_p of (19) one has

$$\tau \partial_p H \left[\gamma(\tau H)^{\gamma-1} - r\tau(\gamma - 1)(\tau H)^{\gamma-2}\right] = 2\sigma^2 p$$

Table 1. Comparison between theoretical and numerical results for the quotient v_γ/v_1. It has been found a maximum deviation of 42% between theoretical and numerical results.

γ	a	$\frac{v_\gamma}{v_1}$ theor	$\frac{v_\gamma}{v_1}$ num
	0.3	0.811	0.723
0.1	0.5	1.317	0.911
	0.7	1.813	1.050
	0.3	0.940	0.847
0.5	0.5	1.379	0.960
	0.7	1.775	1.037
	0.3	1.066	0.967
0.9	0.5	1.412	0.993
	0.7	1.700	1.011

and from (19) one obtains $H = r(3-\gamma)/(2-\gamma)$ and from (18) the linear speed selected by the front is

$$v_\gamma = \frac{\sigma}{\tau}(r\tau)^{1-\frac{\gamma}{2}}(3-\gamma)^{\frac{3-\gamma}{2}}(2-\gamma)^{-1+\frac{\gamma}{2}}. \tag{20}$$

Let us now to explore the interesting properties of this speed. The classical diffusion is recovered for $\gamma = 1$ and therefore the front travels with the Fisher speed

$$v_1 = 2\sigma\sqrt{r/\tau}.$$

In Table 1 we collect the values of the dimensionless speed v_γ/v_1 for different values of the reaction-dispersal dimensionless number $a \equiv r\tau$, which is nothing but the quotient between the characteristic waiting time and the characteristic growth time. Theoretical values obtained from (20) have been compared to the numerical solutions directly performed on equation (8) with $f(\rho) = r\rho(1-\rho)$. The Riemann-Liouville operator (9) is not the best starting point to get the discrete version of the fractional time derivative which will let us to perform numerical integration on equation (8). We use an alternative and equivalent definition of this derivative, namely the Grünwald-Letnikov operator [8] that is more suitable in numerical calculations. In order to get the numerical solution of equation (8) we use the algorithm in reference [11] joint to a classical finite difference scheme for the spatial second derivative. A relatively good agreement between numerical and theoretical results is observed: the maximum deviation found between theoretical and numerical results is 42%.

The theoretical result found in (20) has to fullfil simultaneously some physical restrictions over the subdiffusive range $0 < \gamma \leq 1$. The first one (R1) is that v_γ has to be an increasing function of the reaction rate r and, in consequence, of a. The second one (R2) is that v_γ has to be an increasing function of γ, ranging from 0 to 1, because the transport is faster as γ tends to 1^- and is slower as it tends to 0^+. The third one (R3) is that $v_\gamma < v_1$, because a diffusive transport cannot lead to a front traveling with a speed faster than the corresponding to the classical diffusion v_1. It is easy to check that R1 is always fulfilled. From (20), R2 is fulfilled only if $0 < a \leq 2/3$. In particular, we find that if $0 < a \leq 1/2$, then v_γ is always monotonically increasing with γ for any γ. However, if $1/2 \leq a \leq 2/3$, then

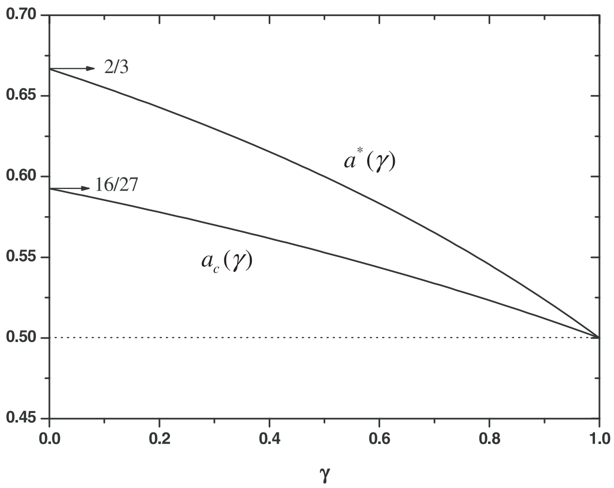

Fig. 1. Plot of the critical curves $a^*(\gamma)$ and $a_c(\gamma)$. It is clear from this figure the results of the physical restriction presented in Table 2. It is observed that R3 is a stronger condition than R2. For $16/27 < a < 2/3$, R2 is fulfilled if $a < a^*(\gamma)$ but R3 is always violated. For $a > 2/3$ both R2 and R3 are violated.

Table 2. Restrictions for the values of a and γ obtained from the three physical restrictions. It is assumed that the transport is always subdiffusive, that is, $0 < \gamma \leq 1$.

Restriction	Allowed values of a and γ
R1 $\left(\frac{\partial v_\gamma}{\partial a} > 0\right)$	any a and any γ
R2 $\left(\frac{\partial v_\gamma}{\partial \gamma} > 0\right)$	$0 < a \leq \frac{1}{2}$ for any γ $\frac{1}{2} < a \leq \frac{2}{3}$ if $a < a^*(\gamma)$
R3 $(v_\gamma < v_1)$	$0 < a \leq \frac{1}{2}$ for any γ $\frac{1}{2} < a \leq \frac{16}{27}$ if $a < a_c(\gamma)$

a and γ have to fulfill the restriction $a < a^*(\gamma)$ where

$$a^*(\gamma) = \frac{2-\gamma}{3-\gamma}. \tag{21}$$

If $a > 2/3$ then R2 is never fulfilled. Finally, from (20), R3 is fulfilled only if $0 < a \leq 16/27$ and in particular, if $0 < a \leq 1/2$ R3 is fulfilled for any γ but if $1/2 \leq a \leq 16/27$ then a and γ have to fulfill the restriction $a < a_c(\gamma)$ where

$$a_c(\gamma) = \left[\frac{4(2-\gamma)^{2-\gamma}}{(3-\gamma)^{3-\gamma}}\right]^{\frac{1}{1-\gamma}}. \tag{22}$$

If $a > 16/27$ then R3 is never fulfilled. In Figure 1 we depict the curves $a^*(\gamma)$ and $a_c(\gamma)$ and may be observed that if R3 is fulfilled then R2 is also automatically fulfilled. In Table 2 we collect the results imposed by the above physical restrictions.

5 Speed of spatial FRD fronts

We compute now the speed of fronts emerging from equation (12). Inserting equations (10) and (11) into (16) one obtains

$$H = \frac{\sigma^{2\alpha}}{\tau} p^{2\alpha} + r. \tag{23}$$

Table 3. Comparison between theoretical and numerical results for the quotient v_α/v_1. It has been found a maximum deviation of 15% between theoretical and numerical results.

α	a	$\frac{v_\alpha}{v_1}$ theor	$\frac{v_\alpha}{v_1}$ num
	0.1	1.69	1.91
0.6	0.5	0.99	1.02
	1	0.79	0.84
	0.1	1.39	1.47
0.75	0.5	1.06	1.05
	1	0.95	0.93
	0.1	1.13	1.16
0.9	0.5	1.03	1.07
	1	0.99	1.03

From (18) we find $H = 2r\alpha/(2\alpha - 1)$ and the front

$$v_\alpha = 2\frac{\sigma}{\tau}\alpha\left(\frac{a}{2\alpha-1}\right)^{1-\frac{1}{2\alpha}} \qquad \text{if} \quad \alpha \geq 1/2. \tag{24}$$

Equation (24) has been recently obtained in reference [4] where the authors have used a linear analysis around the unstable state. Note that the restriction for the existence of a linear speed selected is $\alpha \geq 1/2$. For $\alpha = 1/2$ one has $v_{1/2} = \sigma/\tau$. This is not a surprising result because in this case the transport is driven by advection with a velocity given precisely by σ/τ (see Eq. (12)) and the front travels with the advective velocity. In Table 3 we collect theoretical (computed from (24)) and numerical values of v_α/v_1 for some values of α and a. Numerical solutions have been performed on (12). Discretization of spatial fractional derivative have mainly been made following the methods in reference [12]. As we can see, there are two different algorithms (they call them L2 and L2C) to get the discrete version of the fractional derivative. Moreover, their accuracy depends on the values of the fractional index α. We always have chosen the more accurate one, i.e., L2C method for small values of α and L2 for the large ones. The maximum deviation found, between theoretical and numerical results for the front speed is 15%. So, a good agreement is found.

The three physical restrictions imposed in the previous case, for temporal FRD fronts, may be also considered here in the superdiffusive range $1/2 \leq \alpha \leq 1$. R1 is the same as before: v_α has to be increasing with a. R2 requires that v_α has to be decreasing with α because the transport is faster as $\alpha \to 1/2^+$ (advective limit) and slower as $\alpha \to 1^-$ (classical diffusion limit). As in the previous case, R1 is always fulfilled for any α lying in the range $(\frac{1}{2}, 1)$. R2 is fulfilled if α and a are such that $a < a^*(\alpha)$, where

$$a^*(\alpha) = e^{2\alpha}(2\alpha - 1). \tag{25}$$

R3 requires that the front speed v_α has to be faster than the speed in the classical diffusion limit, v_1. R3 is fulfilled if $0 \leq a \leq 1$. In particular, if $0 \leq a \leq 1/4$ then R3 is always fulfilled, but if $1/4 \leq a \leq 1$ then a and α has to obey the condition $a < a_c(\alpha)$, where

$$a_c(\alpha) = \left[\frac{\alpha^{2\alpha}}{(2\alpha-1)^{2\alpha-1}}\right]^{\frac{1}{1-\alpha}}. \tag{26}$$

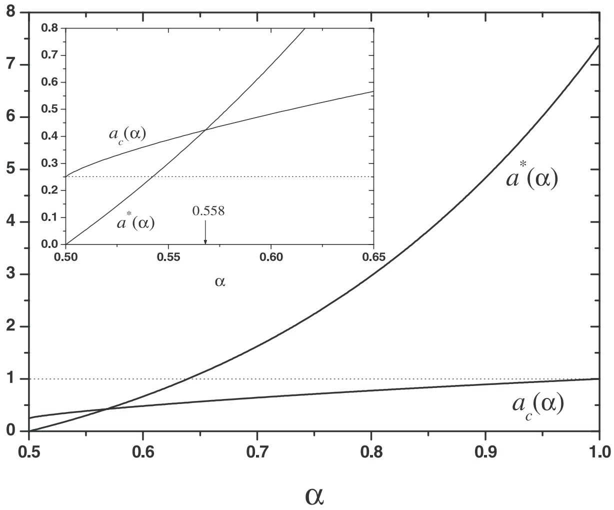

Fig. 2. Plot of the critical curves $a^*(\gamma)$ and $a_c(\gamma)$. It is clear from this figure the results of the physical restriction presented in Table 4. It is observed that R2 is a stronger condition than R3 if $\frac{1}{2} \leq \alpha \leq 0.568$ and R3 is stronger than R2 if $0.568 \leq \alpha \leq 1$. For $1 < a < e^2$, R2 is fulfilled if $a < a^*(\alpha)$ but R3 is always violated while for $a > e^2$ both R2 and R3 are violated.

Table 4. Restrictions for the values of a and α obtained from the three physical restrictions. It is assumed that the transport is always superdiffusive, that is, $\frac{1}{2} < \alpha \leq 1$.

Restriction	Allowed values of a and α
R1 $\left(\frac{\partial v_\alpha}{\partial a} > 0\right)$	any a and any γ
R2 $\left(\frac{\partial v_\alpha}{\partial \alpha} < 0\right)$	$a < a^*(\alpha)$ for any α
R3 $(v_\alpha > v_1)$	$0 < a \leq \frac{1}{4}$ for any α $\frac{1}{4} < a \leq 1$ if $a < a_c(\alpha)$

In Figure 2 we depict the curves $a^*(\alpha)$ and $a_c(\alpha)$ and may be observed that if $1/2 \leq \alpha \leq 0.568$ then R2 implies R3 and if $0.568 \leq \alpha \leq 1$ then R3 implies automatically R2. In Table 4 we collect the results imposed by the physical restrictions.

6 Conclusions

In this work we have proposed the CTRW as a phenomenological model to deal with temporal and spatial anomalous reaction-diffusion equations. We have obtained in a very natural way two different parabolic fractional reaction-dispersal equations that describe anomalous diffusion together with reaction processes. The first one (temporal FRD model) is derived assuming a fractal waiting-time PDF and classical spatial diffusion. The second one (spatial FRD model) assumes a classical waiting-time PDF but a symmetric Lévy flight PDF. Making use of Hamilton-Jacobi analysis, we have been recovered analytic expressions of the linear uniform speed selected for pulled wave fronts, already published. For the first one, the linear speed selection always holds but it fails for the second one if fractional exponent α is lower than 1/2. In both cases we have also checked the validity of our mesoscopic model by means of numerical integrations of the respective equations. We have noticed here that in both cases, the front speed may present a counterintuitive behaviour if reaction-diffusion dimensionless number a is large enough. This is done by requiring that the front speed has to fulfill simultaneously three physical restrictions: R1 (the front speed has to be an increasing function of a), R2 (the front speed has to be an increasing function of γ and a decreasing function of α) and R3 (the front speed v_γ has to be lower than the corresponding to the classical diffusion v_1 and v_α has to be higher than v_1). As a result, we have obtained the corresponding restrictions for values of a, in terms of the fractional indexes γ and α. However, there is still an open question: why do FRD equations, derived within the CTRW scheme, lead to front speeds with unphysical meaning for large a? Some authors have recently detected that this phenomenological description is not adequate to deal with anomalous diffusion with reaction processes [13], although it holds when the waiting-time and spatial PDFs have all the moments finite. They propose new alternative FRD equations but it is not shown if their corresponding front speeds are in agreement with our physical restrictions R1, R2 and R3. On the other hand, it is worthy to note that our numerical results have tested our mesoscopic model but are not able to account for the underlying microscopic processes. Stochastic simulations could be useful to check our results, but this will be the subject of future work.

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