Nonlinear diffusion equation with reaction terms: Analytical and numerical results

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A B S T R A C T

We investigate a process obtained from a combination of nonlinear diffusion equations with reaction terms connected to a reversible process, i.e., $1 \rightarrow 2$, of two species. This feature implies that the species 1 reacts producing the species 2, and vice-versa. A particular case emerging from this scenario is represented by $1 \rightarrow 2$ (or $2 \rightarrow 1$), characterizing an irreversible process where one species produces the other. The results show that in the asymptotic limit of small and long times the behavior of the species is essentially governed by the diffusive terms. For intermediate times, the behavior of the system and particularly the rates depends on the reaction terms. In the presence of external forces, significant changes occur in the asymptotic limits. For these cases, we relate the solutions with the $q$-exponential function of the Tsallis statistic to highlight the compact or long-tailed behavior of the solutions and to establish a connection with the Tsallis thermo-statistic. We also extend the results to the spatial fractional differential operator by considering long-tailed distributions for the probability density function.

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1. Introduction

Diffusion is among the most fascinating phenomena of science, that essentially started with Robert Brown observations of the random motion of particles suspended in a fluid, i.e., pollen grains in water. The same type of motion has been reported in several chemical, physical, and biological processes. Explanations about this type motion appear in pioneering works of Einstein [1], Smoluchowski [2] and Langevin [3]. They have shown, through elegant arguments, how it is possible to model this phenomenon. The main feature about this phenomenon is the linear time dependence of the mean square displacement, i.e., $(\langle \Delta x \rangle^2) \sim t$, which has been related to the Markovian and ergodic properties of these systems. However, several experimental situations have reported effects which are not suitable described in terms of the usual diffusion, such as very fast thermal transients [4], high speed energy transportation, transport through the porous media [5,6], dynamic processes in protein folding [7], infiltration [8], single particle tracking [9], electrical response [10,11], and diffusion on fractals [12]. These situations have motivated extensions of the approaches used to describe standard diffusive processes. One of these

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extensions is the fractional Fokker–Planck equation [13–16], which essentially incorporate fractional differential operators into account [17,18]. Other approaches are the generalized Langevin equations [19,20], continuous time random walks with long-tailed distributions [21] for the probability density function, and the nonlinear Fokker–Planck equations [22–33]. It is worth emphasizing that nonlinear diffusion equations may be related to a thermodynamics [34] characterized by power-law distributions with a compact or a long-tailed behavior, which, in a suitable limit, can be connected to the Lévy distributions [35–37]. They can also be related to other approaches such as Langevin equations [19,20] and random walks.

In several processes, interactions among particles also may occur, in addition to the diffusive phenomena, causing the consumption or production of them. This phenomenon is observed, for example, in chemical reactions, in which the interaction between particles can lead to the conversion of one chemical species to another. The combination of diffusion and reaction processes in a system corresponds to a reaction–diffusion problem [38–40], which was first introduced by Turing [41] to account for the main phenomena of morphogenesis and has been applied in several contexts such as chemical reactions [42], population evolution [43], biological pattern formation [44], epidemics [45], and computer virus spreading [46]. Thus, we have a group of particles (or species) which locally react with each other and globally diffuse in space. This field is vast but lacks a generalized approach for the treatment of this problem as well as the variety of substrates on which such reactions take place [47]. In a sense, our goal here is the analysis of reaction–diffusion processes obtained by considering the nonlinear diffusion equation with reaction terms related to a reversible or irreversible process. We first consider the linear scenario which is next extended to the nonlinear one. In both cases, reaction terms with irreversible or reversible characteristics are considered. The results show that the spreading of the system is essentially governed by the diffusive terms in the asymptotic limit of small and long times. The behavior exhibited for intermediate times is directly affected by the reaction terms. The solutions for the linear case are primarily governed by Gaussians. For the nonlinear case, it can be expressed in terms of power-laws, which may be related to the q-exponentials that are present in the Tsallis statistics [48] and others contexts where generalized thermostatistics are considered [49,50]. These distributions may present a compact or a long tailed behavior as discussed in Refs. [51,52]. In the last case, it can be asymptotically related to the Lévy distributions, which are solutions of the linear fractional diffusion equations [51,53]. In this sense, these distributions are also solutions, in the asymptotic limit, of the linear fractional diffusion equations. By using the Zubarev nonequilibrium statistical operator method and the Liouville equation with fractional derivatives, it is possible to show that these thermostatistics characterized by q – exponentials may be related to a fractional diffusion equation as performed in Ref. [54]. Similar features may be verified when spatial fractional derivatives are incorporated in the nonlinear diffusion equation. It is worth mentioning that it is possible (in the asymptotic limit) to establish a connection between the distributions present in the Tsallis formalism with their solutions by a suitable choice of q as performed in Refs. [55–57]. In this sense, we also analyze the changes produced on the solutions when spatial fractional derivatives are incorporated as a consequence of the long-tailed behavior exhibit by the distributions related to the dispersive term. These analyses are performed in Sections 2 and 3. In Section 4, the discussions and conclusions are presented.

2. Nonlinear diffusion equation

Let us start our discussion by considering the process characterized by the following reaction $1 \rightleftharpoons 2$, where the substrates 1 and 2 may also spread while the reaction process occurs in bulk. Following the development reported in Refs. [58,59], we consider that the reaction process is described by the following balance equations

$$\rho_1(x, t + \tau) = \int_{-\infty}^{\infty} e^{-k_{12}(t)\tau} \Psi_1(\rho_1(x - z, t)) \rho_1(x - z, t) \Phi_1(z)dz$$

$$+ (1 - e^{-k_{12}(t)\tau}) \rho_2(x, t) + e^{-k_{12}(t)\tau} (\rho_1(x, t) - \Psi_1(\rho_1(x, t)) \rho_1(x, t)),$$

$$\rho_2(x, t + \tau) = \int_{-\infty}^{\infty} e^{-k_{21}(t)\tau} \Psi_2(\rho_2(x - z, t)) \rho_2(x - z, t) \Phi_2(z)dz$$

$$+ (1 - e^{-k_{21}(t)\tau}) \rho_1(x, t) + e^{-k_{21}(t)\tau} (\rho_2(x, t) - \Psi_2(\rho_2(x, t)) \rho_2(x, t)),$$

where $k_{12}$ and $k_{21}$ are related to the reaction rates, $\tau$ is a characteristic time, $\Phi_1(\rho_1)$ is a probability density function conveniently normalized, and the dispersal terms consider a nonlinear dependence on the distribution, i.e., $\Psi_1(\rho_1)$ and $\Psi_2(\rho_2)$. They may be used to describe situations characterized by distributions with a compact form or a long-tailed behavior that asymptotically may be connected to the Lévy distributions [60], implying that the diffusion coefficient in each element of the system depends on the history of that element. In addition, different regimes may also emerge from these solutions, depending on the choice of $\Psi(\rho_1)$ and $\Psi(\rho_2)$. The terms related to the reaction process were modified to preserve their linearity; however, by introducing suitable changes, it is possible to obtain nonlinear reaction terms.
Following the developments performed in Ref. [58], by taking into account \( \tau \) and \( z \) sufficiently small when compared to the scales of interest, we may expand the Eqs. (1) and (2) and obtain that

\[
\rho_1(x, t) + \tau \frac{\partial}{\partial t} \rho_1(x, t) \approx \left( 1 - k_{12}(t) \tau \right) \left( \Psi_1(\rho_1) \rho_1(x, t) + \frac{\partial}{\partial x} \left( K_1(\rho_1) \frac{\partial}{\partial x} \rho_1(x, t) \right) \right) + k_{21}(t) \tau \rho_2(x, t) - \left( 1 - k_{12}(t) \tau \right) \left( \Psi_1(\rho_1) \rho_1(x, t) - \rho_1(x, t) \right),
\]

\[
(3)
\]

\[
\rho_2(x, t) + \tau \frac{\partial}{\partial t} \rho_2(x, t) \approx \left( 1 - k_{21}(t) \tau \right) \left( \Psi_2(\rho_2) \rho_2(x, t) + \frac{\partial}{\partial x} \left( K_2(\rho_2) \frac{\partial}{\partial x} \rho_2(x, t) \right) \right) + k_{12}(t) \tau \rho_1(x, t) - \left( 1 - k_{21}(t) \tau \right) \left( \Psi_2(\rho_2) \rho_2(x, t) - \rho_2(x, t) \right),
\]

\[
(4)
\]

where

\[
K_{1(2)}(\rho_{1(2)}) = \frac{\langle z^2 \rangle_{1(2)}}{2} \frac{d}{d\rho_{1(2)}} \left( \Psi(\rho_{1(2)}) \rho_{1(2)} \right)
\]

\[
(5)
\]

and \( \langle z^2 \rangle_{1(2)} = \int_0^\infty 2z^2 \Phi_{1(2)}(z) dz \). The limit \( \tau \to 0 \) and \( z \to 0 \) in the previous set of equations, i.e., in Eqs. (3) and (4), yields

\[
\frac{\partial}{\partial t} \rho_1(x, t) = -k_{12}(t) \rho_1(x, t) \left( \Psi_1(\rho_1) \rho_1(x, t) + k_{21}(t) \rho_2(x, t) \right),
\]

\[
(6)
\]

\[
\frac{\partial}{\partial t} \rho_2(x, t) = -k_{12}(t) \rho_1(x, t) \left( \Psi_2(\rho_2) \rho_2(x, t) + k_{21}(t) \rho_2(x, t) \right),
\]

\[
(7)
\]

with \( K_{1(2)}(\rho_{1(2)}) = K_{1(2)}(\rho_{1(2)}) / \tau \) and \( \langle z^2 \rangle_{1(2)} / \tau \) constant. Later on, we discuss the situation related to the spatial fractional diffusion equation when a long-tailed behavior is incorporated in \( \Phi_1(z) \) and \( \Phi_2(z) \). It is possible to show that \( \int_0^\infty dx \left( \rho_1(x, t) + \rho_2(x, t) \right) \) constant can be verified depending on the choice of \( k_{12}(t) \) and \( k_{21}(t) \), for the boundary conditions \( \rho_1(\pm \infty, t) = 0 \) and \( \rho_2(\pm \infty, t) = 0 \). For this, we may analyze the behavior of the survival probabilities \( S_{1(2)}(t) = \int_0^\infty \rho_{1(2)}(x, t) dx \) related to \( \rho_1(x, t) \) and \( \rho_2(x, t) \) which satisfy the following set of equations:

\[
\frac{d}{dt} S_1(t) = k_{21}(t) S_2(t) - k_{12}(t) S_1(t),
\]

\[
(8)
\]

\[
\frac{d}{dt} S_2(t) = k_{12}(t) S_1(t) - k_{21}(t) S_2(t).
\]

(9)

The solutions obtained from this set of equations are given by

\[
S_1(t) = S_1(0) e^{-\int_0^t k_1(t') dt'}
\]

\[
+ \left( S_1(0) + S_2(0) \right) \int_0^t dt' k_{21}(t') e^\int_0^{t'} dt" \partial \Phi_k(t") e^{-\int_0^t dt" \partial \Phi_k(t")},
\]

(10)

and

\[
S_2(t) = S_2(0) e^{-\int_0^t k_2(t') dt'}
\]

\[
+ \left( S_1(0) + S_2(0) \right) \int_0^t dt' k_{12}(t') e^\int_0^{t'} dt" \partial \Phi_k(t") e^{-\int_0^t dt" \partial \Phi_k(t")},
\]

(11)

with \( k_1(t) = k_{12}(t) + k_{21}(t) \). Eqs. (10) and (11) show that, for long times with \( k_{12}(t) \to k_{12} = \text{constant} \) and \( k_{21}(t) \to k_{21} = \text{constant} \), the reaction process reaches a state of equilibrium with \( S_1 \to k_{21}/k_1 \) and \( S_2 \to k_{12}/k_1 \). The results obtained for \( S_1 \) and \( S_2 \) are independent of the diffusive terms \( K_1(\rho_1) \) and \( K_2(\rho_2) \) and depend on the rates \( k_{12}(t) \) and \( k_{21}(t) \), which determine the formation of the species 2 and 1. If one of the diffusive terms is absent, e.g., \( K_2(\rho_2) = 0 \), the results obtained for \( S_1 \) and \( S_2 \) imply an interchange between the states of motion and pauses when the system is diffusing on a substrate, as discussed in Ref. [59].

3. Time dependent solutions

Now, we analyze some cases related to Eqs. (6) and (7) by using analytical or numerical approaches. We start our analysis by considering the case \( \Psi_{1(2)}(\rho_{1(2)}) = 1 \), which implies that the diffusion process is usual and asymptotically characterized by a linear time dependence for the mean square displacement. For this case, it is possible to obtain exact solutions by using the standard calculus techniques. In particular, for the case \( k_{12}(t) = k_{12} = \text{constant} \) and \( k_{21}(t) = k_{12} = \text{constant} \)
subjected to the boundary conditions \( \rho_1(\pm \infty, t) = 0 \) and \( \rho_2(\pm \infty, t) = 0 \) and the initial conditions \( \rho_1(x, 0) = \psi(x) \) and \( \rho_2(x, 0) = 0 \), the solutions can be found by using integral transforms, i.e., the Fourier and Laplace transforms. By using the Fourier transform in Eqs. (6) and (7), we obtain

\[
\frac{\partial}{\partial t} \rho_1(k, t) = -k^2 K_1 \rho_1(k, t) - k_{12} \rho_1(k, t) + k_{21} \rho_2(k, t),
\]

(12)

\[
\frac{\partial}{\partial t} \rho_2(k, t) = -k^2 K_2 \rho_2(k, t) + k_{12} \rho_1(k, t) - k_{21} \rho_2(k, t).
\]

(13)

By applying the Laplace transform in Eqs. (12) and (13), it is possible simplify them to the following equations

\[
s \rho_1(k, s) - \rho_1(k, 0) = -k^2 K_1 \rho_1(k, s) - k_{12} \rho_1(k, s) + k_{21} \rho_2(k, s).
\]

(14)

\[
s \rho_2(k, s) = -k^2 K_2 \rho_2(k, s) + k_{12} \rho_1(k, s) - k_{21} \rho_2(k, s).
\]

(15)

After some calculations, the solution for \( \rho_1(k, s) \) and \( \rho_2(k, s) \), i.e., in the Fourier and Laplace domain, is given by

\[
\rho_1(k, s) = \frac{(s + k^2 K_2 + k_{21}) \rho_1(k, 0)}{(s + k^2 K_1)(s + k^2 K_2 + k_{21}) + k_{12}(s + k^2 K_2)},
\]

(16)

\[
\rho_2(k, s) = \frac{k_{12} \rho_1(k, 0)}{(s + k^2 K_1)(s + k^2 K_2 + k_{21}) + k_{12}(s + k^2 K_2)}.
\]

(17)

Now, let us perform the inverse Fourier and Laplace transforms. For this, we may use the following expansion

\[
\Pi_n(k, s) = \left(k_{12} - \frac{k_{12} k_{21}}{s + k^2 K_2 + k_{21}}\right)^n (s + k^2 K_2 + k_{21}) + s + k^2 K_2 = \sum_{n=0}^{\infty} \frac{(-1)^n}{(s + k^2 K_1)^{n+1}} \Pi_n(k, s),
\]

yielding for \( \rho_1(x, t) \) and \( \rho_2(x, t) \) the following expressions

\[
\rho_1(x, t) = \int_{-\infty}^{\infty} dx' G(x - x', t) \psi(x),
\]

(18)

and

\[
\rho_2(x, t) = \int_0^t dt' \int_{-\infty}^{\infty} dx' G^{(2)}(x - x', t - t'; k_2) \rho_1(x', t'),
\]

(19)

with

\[
G(x, t) = G^{(1)}(x, t) + \sum_{n=1}^{\infty} (-1)^n \int_0^t dt_n \int_{-\infty}^{\infty} dx_n G^{(3)}(x - x_n, t - t_n; k_2) \times \int_0^{t_n} dt_n \int_{-\infty}^{\infty} dx_n G^{(3)}(x_n - x_{n-1}, t_n - t_{n-1}; k_2) \ldots \times \int_0^{t_1} dt_1 \int_{-\infty}^{\infty} dx_1 G^{(3)}(x_1 - x_2, t_1 - t_2; k_2) G^{(1)}(x_1, t_1).
\]

(20)

\[
G^{(3)}(x, t) = k_{12} G^{(1)}(x, t)
\]

\[
- k_{12} k_{21} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{t} dt' G^{(1)}(x - x', t - t') G^{(2)}(x', t'; k_{21}) dt'.
\]

(21)

where

\[
G^{(1)}(x, t) = \frac{1}{\sqrt{4\pi K_1 t}} e^{-x^2/(4K_1 t)}
\]

(22)

and

\[
G^{(2)}(x, t; k_{21}) = \frac{1}{\sqrt{4\pi K_2 t}} e^{-k_{21} t / 4K_2 t} e^{-x^2/(4K_2 t)}.
\]

(23)
For the case $K_1 = K_2 = K$, with the boundary conditions $\rho_1(\pm \infty, t) = 0$ and $\rho_2(\pm \infty, t) = 0$, Eqs. (12) and (13) can be written as

$$\frac{\partial}{\partial t} \rho_1(k, t) = -k^2 \kappa \rho_1(k, t) - k_{12}(t) \rho_1(k, t) + k_{21}(t) \rho_2(k, t),$$

$$\frac{\partial}{\partial t} \rho_2(k, t) = -k^2 \kappa \rho_2(k, t) + k_{12}(t) \rho_1(k, t) - k_{21}(t) \rho_2(k, t),$$

which for the initial conditions $\rho_1(x, 0) = \varphi_1(x)$ and $\rho_2(x, 0) = \varphi_2(x)$, leads us to obtain

$$\rho_1(k, t) = \varphi_1(k) e^{-k^2 \kappa t} e^{-\int_0^t dt' k_1(t')}$$

$$+ \left. e^{-\int_0^t dt' k_1(t')} \right|_0^t \int_0^t dt' k_2(t') \varphi_1(k) + \varphi_2(k) e^{-k^2 \kappa t} e^{-\int_0^t dt' k_1(t')},$$

$$\rho_2(k, t) = \varphi_2(k) e^{-k^2 \kappa t} e^{-\int_0^t dt' k_1(t')}$$

$$+ \left. e^{-\int_0^t dt' k_1(t')} \right|_0^t \int_0^t dt' k_{12}(t') \varphi_1(k) + \varphi_2(k) e^{-k^2 \kappa t} e^{-\int_0^t dt' k_1(t')},$$

with $k_1(t)$ defined as before. From the previous set of equations, by performing the inverse of Fourier transform it is possible to obtain that $\rho_1(x, t)$ and $\rho_2(x, t)$ and they are given by

$$\rho_1(x, t) = e^{-\int_0^t dt' k_1(t')} \int_{-\infty}^{\infty} d\chi \varphi_1(\chi)$$

$$+ \left. \int_{-\infty}^{\infty} d\chi \varphi_1(\chi) \right|_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\chi \Lambda(\chi) k_2(t) e^{-\int_0^t dt' k_1(t')}$$

and

$$\rho_2(x, t) = e^{-\int_0^t dt' k_1(t')} \int_{-\infty}^{\infty} d\chi \varphi_2(\chi)$$

$$+ \left. \int_{-\infty}^{\infty} d\chi \varphi_2(\chi) \right|_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\chi \Lambda(\chi) k_1(t) e^{-\int_0^t dt' k_1(t')}$$

with $\Lambda(x) = \varphi_1(x) + \varphi_2(x)$ (see Fig. 1).

Similar equations have been used to investigate the experimental results of heat conduction in nanofluid suspensions where transient processes are present \[61–63\] and diffusion process of solute in soil \[64,65\]. It is important to observe the presence of exponential (Gaussian) kernels in Eq. (14), which are an important feature of usual diffusion processes.

For the case $\Psi(\rho_{1(2)}) = \rho_{1(2)}^{\gamma_{1(2)}-1}$, we obtain the following differential equations:

$$\frac{\partial}{\partial t} \rho_1(x, t) = K_1 \frac{\partial^2}{\partial x^2} \rho_1^{\gamma_1}(x, t) - k_{12}(t) \rho_1(x, t) + k_{21}(t) \rho_2(x, t),$$

$$\frac{\partial}{\partial t} \rho_2(x, t) = K_2 \frac{\partial^2}{\partial x^2} \rho_2^{\gamma_2}(x, t) + k_{12}(t) \rho_1(x, t) - k_{21}(t) \rho_2(x, t).$$

Fig. 1. These figures illustrate the behavior of the mean square displacement, Fig. 1A, and the solutions $\rho_1(x, t)$, Fig. 1B, and $\rho_2(x, t)$, Fig. 1C, obtained from Eqs. (18) and (19). For simplicity, we also consider $\rho_1(x, 0) = \delta(x)$, $\rho_2(x, 0) = \delta(x)$, $k_{12}(t) = k_{21}(t)/5 = 10^{-5} [T]^{-1}$, and $K_1 = K_2 = 1 [L]^2[T]^{-1}$ where $[L]$ and $[T]$ represent arbitrary units of length and time.
In these equations, the diffusive terms have a nonlinear dependence on the distributions \( \rho_1(x, t) \) and \( \rho_2(x, t) \), characteristic of an anomalous correlated diffusion [34] and chemotaxis of biological population [66]. This feature can be connected with the Tsallis statistics that is based on the following entropy [34,67]:

\[
S_q = \frac{k}{q-1} \left( 1 - \int_0^\infty dx \rho^q \right),
\]

(32)

where the index \( q \) represents a degree of nonextensivity of the system [34] and \( q \to 1 \) recovers the Boltzmann–Gibbs entropy, Eqs. (30) and (31) in the absence of reaction terms have been applied in several situations such as percolation of gases through porous media [68], thin saturated regions in porous media, thin liquid films spreading under gravity [69], and solid-on-solid model for surface growth [70] and superconductors [71]. When the reaction terms are considered, Eqs. (30) and (31) describe a diffusion process of \( 1 \to 2 \) and allow the analysis of the mechanism of chemical diffusion in solids and liquids [72–74]. Also, nonlinear diffusion equations with reaction terms have also been used to analyze the formation of chemical compounds such as NH₄Cl [48], unimolecular reactions [75,76], and the hydroxyl radical reaction with molecular hydrogen for plant respiration [75,76].

For the case \( k_{21}(t) = 0 \), i.e., only one species is formed by the reaction process \( 1 \to 2 \), we may also obtain a formal solution for the previous set of equations for the case \( v_2 = 1 \) by considering the boundary conditions \( \rho_1(\pm \infty, t) = 0 \) and \( \rho_2(\pm \infty, t) = 0 \), for the initial conditions \( \rho_1(x, 0) = \delta(x) \) and \( \rho_2(x, 0) = 0 \). In particular, for this case, following the procedure used in Refs. [77,78], it is possible to verify that

\[
\rho_1(x, t) = e^{-\frac{\beta}{\rho} dt k_{12}(t')} \exp_{\rho_1} \left[ -\beta(t) x^2 \right] \int Z(t),
\]

(33)

and

\[
\rho_2(x, t) = \int_{-\infty}^\infty \int_0^t G^{(2)}(x - x', t - t'; 0) \times \frac{1}{\sqrt{Z(t')}} \rho_{12}(t) e^{-\frac{\beta}{\rho} dt k_{12}(t')} \exp_{\rho_1} \left[ -\beta(t') x'^2 \right] dx' dt',
\]

(34)

with \( v_1 = 2 - q \), \( \frac{\beta(t)}{\rho} = \int_0^\infty \int_0^t e^{-\frac{\beta}{\rho} dt k_{12}(t')} \exp_{\rho_1} \left[ -\beta(t') x^2 \right] dx' dt' \),

\[
\beta(t) = 1 \left\{ 2 v_1 (1 + v_1) Z^{(0)}(q_1) \right\}^{q_1 - 1} \int_0^t dt' e^{(1 - v_1) \frac{\beta}{\rho} dt k_{12}(t')},
\]

(35)

where \( Z^{(n)}(q_1) = \int_{-\infty}^\infty x^n \exp_{\rho_1} \left[ -x^2 \right] dx \), and \( \exp_{\rho_1}[x] \) are the q-exponential functions present in the Tsallis statistics, defined as follows:

\[
\exp_{\rho_1}[x] = \begin{cases} (1 + (1 - q)x)^{1/(1-q)}, & x > 1/(1-q), \\ 0, & x < 1/(1-q). \end{cases}
\]

(36)

The presence of the q-exponential in Eqs. (33) and (34) enables us to obtain a short \( q < 1 \) or a long \( q > 1 \) tailed behavior for the solution depending on the choice of the parameter q. In fact, Eq. (33) has a compact behavior for q less than one due to the cut-off manifested by the q-exponential to retain the probabilistic interpretation associated to \( \rho_1(x, t) \), i.e., we obtain \( \rho_1(x, t) \geq 0 \) if Eq. (36) is satisfied. Consequently, \( \rho_2(x, t) \) is influenced by the behavior of \( \rho_1(x, t) \) when q is less than one. On the other hand, for q greater than one, Eq. (33) has the asymptotic limit governed by a power-law behavior, which may also be related to a Lévy distribution, as shown in [60]. In this case, the solutions obtained for the previous set of equations may be asymptotically related to the solutions obtained in [79] for fractional diffusion equations, which are asymptotically governed by power-laws. It is important to stress that the presence of power-law-based functions represents evidence that the diffusion process is anomalous.

The mean square displacement related to the distribution \( \rho_1(x, t) \) is given by

\[
(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle_1 = e^{-\frac{\beta}{\rho} dt k_{12}(t')} \int Z^{(0)}(q_1) \beta(t) dt,
\]

(37)

which, for small times with \( k_{12}(t) = k_{12} \) constant, i.e., \( t \ll k_{12} \), \( (\Delta x)^2 \sim t^{2/(3-q_1)} \) and, for long times, i.e., \( t \to \infty \), yields \( \langle (\Delta x)^2 \rangle_1 \to 0 \). For \( \rho_2(x, t) \), we have that

\[
(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle_2 = 2 k_2 \left( t - \int_0^t dt e^{-\frac{\beta}{\rho} dt k_{12}(t')} \right) + \int Z^{(2)}(q_1) \int_0^t dt' k_{12}(t') \int_0^t dt e^{\frac{\beta}{\rho} dt k_{12}(t')} \left[ \frac{1}{\beta(t)} \right],
\]

(38)

which for small times has the asymptotic limit \( (\Delta x)^2 \sim t^{(5-q_1)/(3-q_1)} \) and for long times is asymptotically characterized by \( (\Delta x)^2 \sim t \) for \( v > 1 \). The case \( k_2 \to 0 \) leads us to \( (\Delta x)^2 \) constant for long times, characterizing that, for long times, all the particles obtained from the reaction process are switched from the diffusive mode to the resting mode.
Fig. 2. These figures illustrate the behavior of the mean square displacement, Fig. 2A, obtained from Eqs. (30) and (31) and the distributions $\rho_1(x, t)$, Fig. 2B, and $\rho_2(x, t)$, Fig. 2C, for $v_1=1.5$. For simplicity, we consider $\rho_1(x, 0) = \delta(x)$, $\rho_2(x, 0) = 0$. $k_{12}(t) = k_{21}(t) = 10^2 [T]^{-1}$, $K_1 = 1 [L]^{1+\nu_1}[T]^{-1}$, and $K_2 = 1 [L]^{1+\nu_2}[T]^{-1}$, where [L] and [T] represent arbitrary units of length and time.

Fig. 3. These figures illustrate the behavior of the mean square displacement and the survival probabilities obtained from Eqs. (30) and (31) for distributions $\rho_1(x, t)$ and $\rho_2(x, t)$ by considering $v_1=1.5$ and $v_2=1.0$. Fig. 3A considers the initial conditions $\rho_1(x, 0) = \delta(x)$, $\rho_2(x, 0) = 0$. For Fig. 3B, we consider the initial conditions $\rho_1(x, 0) = \delta(x)$, $\rho_2(x, 0) = \delta(x)$. Fig. 3C shows the survival probability related to Fig. 3A ($S_{1,1}(t)$ and $S_{2,1}(t)$) and B (represented by $S_{1,2}(t)$ and $S_{2,2}(t)$). In particular, it evidences an initial transient for $\rho_2(x, t)$ when the species 2 is initially absent. For simplicity, we consider, $k_{12}(t) = 10^2 e^{-t} [T]^{-1}$, $k_{21}(t) = 10^2 e^{-2t} [T]^{-1}$, $K_1 = 1 [L]^{1+\nu_1}[T]^{-1}$, and $K_2 = 1 [L]^{1+\nu_2}[T]^{-1}$, where [L] and [T] represent arbitrary units of length and time.

Fig. 4. These figures illustrate the behavior of the mean square displacement, Fig. 4A, obtained from Eqs. (30) and (31) and the distributions $\rho_1(x, t)$, Fig. 4B, and $\rho_2(x, t)$, Fig. 4C, for $v_1=0.8$ and $v_2=1.0$. For simplicity, we consider $\rho_1(x, 0) = \delta(x)$, $\rho_2(x, 0) = 0$. $k_{12}(t) = k_{21}(t) = 10^2 [T]^{-1}$, $K_1 = 1 [L]^{1+\nu_1}[T]^{-1}$, and $K_2 = 1 [L]^{1+\nu_2}[T]^{-1}$, where [L] and [T] represent arbitrary units of length and time.

For a general situation, i.e., $v_1$ and $v_2$ arbitrary, it is possible to obtain more information about the behavior of the mean square displacement and the distributions $\rho_1(x, t)$ and $\rho_2(x, t)$ by performing numerical calculations. In fact, by using the numerical algorithms based on central differences [80], it is possible to numerically solve Eqs. (30) and (31) that are coupled by the reaction terms, where for simplicity $k_{12}(t) = k_{12} = \text{constant}$ and $k_{21}(t) = k_{21} = \text{constant}$. Fig. 2 shows the behavior of $(\Delta x)^2_1$ and $(\Delta x)^2_2$ for $v_1=1.5$ and $v_2=1$, leading to an interplay between two different diffusion processes which for long times is asymptotically governed by the diffusive term with the long-tailed distribution. In this case, the asymptotic behavior is governed by $v_2=1$ since that $v_1=1.5$ has a compact behavior. It is worth mentioning that for small times the species 1 manifests a sub-diffusive behavior due to the nonlinearity present in Eq. (30) and the species 2 shows a transient due to the choice of the initial condition. In this figure, $\rho_1(x, t)$ is also illustrated for different times. Fig. 3 illustrates the behavior of the mean square displacement and the survival probabilities obtained from Eqs. (30) and (31) for different initial conditions when time-dependent reaction terms are considered. A similar analysis is performed in Fig. 4.
For the case characterized by the parameters \( v_1 = 0.8 \) and \( v_2 = 1 \), which in the asymptotic limit of long times leads us an anomalous diffusion. Figs. 2–4 were obtained by solving numerically Eqs. (30) and (31). For this, the system was defined in the interval \([-5000, 5000]\) and discretized in increments of \( dx = 2 \times 10^{-2} \) with \( dt = 10^{-6} \) to perform numerically the time evolution and obtain the results presented in these figures. These choices for \( dx \) and \( dt \) verify the condition \( k dt/(dx^2) < 1/2 \) required for the stability of the solutions during the time evolution of the initial condition in order to satisfy the boundary conditions [81]. Another interesting point about these figures concerns the time evolution of the solution when small times are considered, they show that \( \rho_2(x, t) \) initially increases and, after, it spreads while reaches the equilibrium, i.e., \( k_{12} \rho_1(x, t) \approx k_{21} \rho_2(x, t) \). These considerations were also applied in the numerical calculations performed to obtain the other figures.

In order to investigate the behavior of the solutions in the asymptotic limit of long times in this scenario, we may analyze the following equation:

\[
\frac{\partial}{\partial t}(\rho_1(x, t) + \rho_2(x, t)) = \mathcal{K}_1 \frac{\partial^2}{\partial x^2} \rho_1^{\nu_1}(x, t) + \mathcal{K}_2 \frac{\partial^2}{\partial x^2} \rho_2^{\nu_2}(x, t),
\]

which can be obtained from the previous set of equations. For \( t \to \infty \), by taking into account \( \rho_2(x, t) \approx (k_{12}/k_{21}) \rho_1(x, t) \), this equation can be approximated to

\[
\frac{\partial}{\partial t}(\rho_1(x, t)) \approx \mathcal{K}_1 \frac{\partial^2}{\partial x^2} P_1^{\nu_1}(x, t) + \mathcal{K}_2 x \frac{\partial^2}{\partial x^2} P_1^{\nu_1}(x, t),
\]

where \( \mathcal{K}_1 = k_{21} \mathcal{K}_1/(k_{12} + k_{21}) \), \( \mathcal{K}_2 = k_{21} \mathcal{K}_2/(k_{12} + k_{21}) \), and \( \alpha = (k_{12}/k_{21})^{\nu_2}. \)

Eq. (40) evidences that the solution may exhibit different regimes depending on the choice of \( \nu_1 \) and \( \nu_2 \) as discussed in Ref. [82]. We can express the solutions given in terms of the \( q \)-exponential functions. For example, for the case \( \nu_1 = \nu_2 = \nu \), after performing some calculations, it is possible to show that the solution can be written as

\[
\rho_1(x, t) \approx \exp_q \left[ -\beta(t)x^2 \right] Z(t),
\]

with \( \nu = 2 - q \), \( \mathcal{K} = \mathcal{K}_1 + \alpha \mathcal{K}_2 \), \( \beta(t) \sqrt{\beta(t)} = T^{(0)}(q) = [(k_{21} + k_{12})/k_{21}] T^{(0)}(q) \).

\[
\beta(t) = 1/\left[ 2\nu(1 + \nu)KZ^{(0)}(q) \right]^{\nu-1} t^{\nu}. \]

Fig. 5 illustrates the solutions obtained numerically (black lines) and the approximated ones (red lines) obtained from Eq. (40), to show that we have a complete agreement among them for long times.

In presence of external forces, Eqs. (30) and (31) are given by

\[
\frac{\partial}{\partial t} \rho_1(x, t) = \mathcal{K}_1 \frac{\partial^2}{\partial x^2} \rho_1^{\nu_1}(x, t) - \frac{\partial}{\partial x} \left[ F_1(x, t) \rho_1(x, t) \right] - k_{12}(t) \rho_1(x, t) + k_{21}(t) \rho_2(x, t),
\]
Nonlinear example, in this force $F_1(t) = -k_1 x$. We also illustrate the time behavior of Eq. (43) in Fig. 6B. For simplicity, we consider $k_{12}(t) = k_{21}(t) = 10^{2} \left[ T \right]^{-1}$, $k_{1} = 1 \left[ l \right]^{-1}$, and $k_{2} = 1 \left[ l \right]^{-1}$, where $[l]$ and $[T]$ represent arbitrary units of length and time.

\[
\frac{\partial}{\partial t} \rho_2(x, t) = K_2 \frac{\partial^2}{\partial x^2} \rho_2^{(2)}(x, t) - \frac{\partial}{\partial x} \left[ F_2(x, t) \rho_2(x, t) \right] + k_{12}(t) \rho_1(x, t) - k_{21}(t) \rho_2(x, t). \tag{44}
\]

which can be approximated to

\[
\frac{\partial}{\partial t} \rho_1(x, t) \approx K_1 \frac{\partial^2}{\partial x^2} \rho_1^{(1)}(x, t) + \alpha \frac{\partial^2}{\partial x^2} \rho_1^{(2)}(x, t)
\]

\[
\quad - \tilde{k} \frac{\partial}{\partial x} \left[ F_1(x, t) + \frac{k_{12}}{k_{21}} F_2(x, t) \right] \rho_1(x, t) \tag{45}
\]

for $k_{12}(t) = k_{12} = \text{constant}$ and $k_{21}(t) = k_{21} = \text{constant}$ with $\tilde{k} = k_{21} / (k_{12} + k_{21})$. when the reaction terms reach the equilibrium, i.e., $\rho_2(x, t) = (k_{12}/k_{21}) \rho_1(x, t)$ as in the previous case. Eq. (45) has as stationary solution

\[
\tilde{K}_1 \ln \rho_1(x) + \alpha \tilde{K}_2 \ln \rho_2, \rho_1(x) = -V_1(x) - \left( k_{12}/k_{21} \right) V_2(x) \tag{46}
\]

which for $v_1 = v_2 = v$ is given by

\[
\rho_1(x) \propto \exp \left\{ -V_1(x)/\tilde{K} - \left( k_{12}/k_{21} \right) V_2(x)/\tilde{K} \right\}. \tag{47}
\]

Other choices for $\Psi_1(\rho_1)$ and $\Psi_2(\rho_2)$ are also possible – in particular, $\Psi_1(\rho_1) = 1 + (\tilde{K}/\tilde{K}_1)(\rho_1)^{-1}$, which may be related to different diffusive behaviors, one characterized by an usual diffusion and the other by an anomalous one. This choice for $\Psi_1(\rho_1)$ found applications, for example, in the spatial diffusion of dispersing animals [81,83] and in overdamped motion of interacting particles [84]. It is worth mentioning that $\Phi(x)$ also has a direct influence on the diffusion process and a different choice for this distribution also leads to different behaviors for the solutions. In particular, scenarios related to spatial fractional time derivatives require a power-law dependence for this distribution. In fact, for example, for the linear case, by considering $\Phi_1(\rho_1) \propto 1/|z|^{1+\mu_1/2}$, it is possible to obtain situations worked out in Ref. [85], where fractional spatial derivative is present. In this context, a general scenario may be obtained by incorporating a nonlinear dependence in $\Psi_2(\rho_2)$ yielding, for example,

\[
\frac{\partial}{\partial t} \rho_1(x, t) = K_1 \frac{\partial^{\mu_1}}{\partial |x|^\mu_1} \rho_1^{(1)}(x, t) - k_{12}(t) \rho_1(x, t) + k_{21}(t) \rho_2(x, t), \tag{48}
\]

\[
\frac{\partial}{\partial t} \rho_2(x, t) = K_2 \frac{\partial^{\mu_2}}{\partial |x|^\mu_2} \rho_2^{(2)}(x, t) + k_{12}(t) \rho_1(x, t) - k_{21}(t) \rho_2(x, t). \tag{49}
\]

where $\frac{\partial^{\mu}}{\partial |x|^\mu}$ is a fractional spatial operator in the Riesz–Wely sense [17]. Fig. 7 illustrates the behavior of Eqs. (48) and (49) for different times for the initial conditions $\rho_1(x, 0) = \delta(x)$ and $\rho_2(x, 0) = 0$. In this figure, we also illustrate the behavior of $\rho_1(0, t)$ and $\rho_2(0, t)$ as a qualitative measure of the spreading of the system. Fig. 8 illustrates the time evolution of $\rho_1(x, t)$ and $\rho_2(x, t)$ by taking into account the initial conditions $\rho_1(x, 0) = \delta(x)$ and $\rho_2(x, 0) = 0$. It is also illustrated the behavior of $\rho_1(0, t)$ and $\rho_2(0, t)$. In this point, it should be mentioned that the numerical calculations were performed following the approach presented in Refs. [86,87] for the fractional differential operators. Similar to the results presented in Fig. 7, we observe that for long times $\rho_1(0, t)$ and $\rho_2(0, t)$ manifest the same time dependence, indicating that for long times an equilibrium is reached, i.e., $k_{12} \rho_1(x, t) \approx k_{21} \rho_2(x, t)$ when $k_{12}(t) = k_{12} = \text{constant}$ and $k_{21}(t) = k_{21} = \text{constant}$. In
Fig. 7. Behavior of Eqs. (48) and (49) by considering the initial condition \( \rho_1(x, 0) = \delta(x) \) and \( \rho_2(x, 0) = 0 \) with \( v_1 = 1.3 \) and \( \mu_1 = 1.8 \). For simplicity, we consider \( k_{12}(t) = k_{21}(t) = 10^2 \ T^{-1} \), \( K_1 = 1 \ [L]^{n+1-1} \ T^{-1} \), and \( K_2 = 0 \). where [L] and [T] represent arbitrary units of length and time.

![Graph A](image1.png)

![Graph B](image2.png)

Fig. 8. Behavior of Eqs. (48) and (49) is illustrated in Fig. 8A by considering the initial condition \( \rho_1(x, 0) = \delta(x) \) and \( \rho_2(x, 0) = \delta(x) \) with \( v_1 = 1.3 \), \( \mu_1 = 1.8 \), \( v_2 = 1 \), and \( \mu_2 = 2 \). Fig. 8B shows the spreading of the distributions through the behavior of \( \rho_1(0, t) \) and \( \rho_2(0, t) \). For simplicity, we consider \( k_{12}(t) = k_{21}(t) = 10^2 \ T^{-1} \), \( K_1 = 1 \ [L]^{n+1-1} \ T^{-1} \), and \( K_2 = 1 \ [L]^{2} \ T^{-1} \), where [L] and [T] represent arbitrary units of length and time.

![Graph C](image3.png)

![Graph D](image4.png)

particular, when the equilibrium is reached the following approximation may be verified:

\[
\frac{\partial}{\partial t} \rho_1(x, t) \approx \overline{K}_1 \frac{\partial^{\mu_1}}{\partial |x|^{\mu_1}} \rho_1(x, t) + \alpha \overline{K}_2 \frac{\partial^{\mu_2}}{\partial |x|^{\mu_2}} \rho_1^2(x, t).
\] (50)

Eq. (50) may manifest different behaviors depending on the choice of the parameters \( v_1 \), \( v_2 \), \( \mu_1 \), and \( \mu_2 \). In addition, for the case \( v_1 = v_2 = 1 \) with \( \mu_1 \neq 2 \) and \( \mu_2 \neq 2 \), it has the solution given by

\[
\rho_1(x, t) = \overline{K} \sum_{n=0}^{\infty} \frac{(-\overline{K} t)^n}{\Gamma(1+n)}
\times \int_{-\infty}^{\infty} dx \frac{\rho_1(x, 0)}{|x - x'|^{1+\mu_1}} H_{1.1, 2}^{2, 1}
\left|
\begin{array}{ccc}
|x|^{\mu_1} & (1.1, (1+\frac{\mu_1}{2}, \frac{\nu_1}{2})) \\
\overline{K} t & (1+\mu_1, 1+\frac{\nu_1}{2})
\end{array}
\right|
\]

(51)

where \( H[\ldots] \) is the Fox H-function [89].

4. Discussions and conclusions

We analyzed a nonlinear reaction–diffusion equation by considering different scenarios. Our analysis started by considering balance equations with nonlinear dependence on the dispersal terms. For the reaction terms, we also considered a suitable choice to preserve the linearity of them. For the diffusion equations which emerge from these balance equations, we showed the mass conservation and that after some time an equilibrium is reached. For these equations, we also obtained the analytical or numerical solutions. The analytical solutions were obtained for the linear case \( v_1 = v_2 = 1 \) with \( k_{12} = 0 \) and \( k_{21} = 0 \). For the case \( v_1 \neq 1 \) and \( v_2 = 1 \) with \( k_{12} = 0 \) and \( k_{21} = 0 \), we also obtained a solution. In particular, for the last case, \( q \)-exponentials functions present in the Tsallis statistics were used to obtain the exact time-dependent solutions. We verified for this case that, depending on the choice of the parameter \( v_1 \), the solution may exhibit a compact or a long-tailed behavior, which may be connected to a subdiffusion or superdiffusion process. For the case \( k_{12} = 0 \) with \( k_{21} = 0 \), which implies in an interchange between the two species, we performed a numerical analysis and verified that, for small and long times, the behavior of \( \rho_1(x, t) \) was essentially characterized by a diffusive behavior and for \( \rho_2(x, t) \) a transient
was initially observed. For intermediate times, the reaction terms played an important role, and the system exhibits for each species a different diffusive regime from the initial one. After, we obtained some approximated results for $\rho_1(x, t)$ and $\rho_2(x, t)$ when long times are considered. In particular, we showed that the distributions which represent the species are governed by Eq. (40) when the condition $k_{21}P_2(x, t) \approx k_{12}P_1(x, t)$ is satisfied. Following, we have analyzed the influence of external forces on the solutions and shown that a stationary solution can be found depending on the choice of $F_1(x, t)$ and $F_2(x, t).$ Other choices for $\Psi_{1/2}^{(1/2)}$ and $F_{1/2}(x, t)$ lead us to different behaviors from the ones reported here. We also discussed one of the possible consequences which emerge when different choices for the distribution $\Psi_{1/2}^{(1/2)}$ are performed. In particular, one of them may lead to a fractional diffusion equation with the spatial fractional derivatives whose solutions may be related to the Lévy distributions and may exhibit different regimes of diffusion.

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References