



Nonlinear diffusion equation with reaction terms: Analytical and numerical results

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ABSTRACT

We investigate a process obtained from a combination of nonlinear diffusion equations with reaction terms connected to a reversible process, i.e., $1 \rightleftharpoons 2$, 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., $\langle (\Delta x)^2 \rangle \sim t$, 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 thermostatics 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 thermostatics 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 substances 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

$$\begin{aligned} \rho_1(x, t + \tau) = & \int_{-\infty}^{\infty} e^{-k_{12}(t)\tau} \Psi_1(\rho_1(x - z, t)) \rho_1(x - z, t) \Phi_1(z) dz \\ & + (1 - e^{-k_{21}(t)\tau}) \rho_2(x, t) \\ & + e^{-k_{12}(t)\tau} (\rho_1(x, t) - \Psi_1(\rho_1(x, t)) \rho_1(x, t)), \end{aligned} \tag{1}$$

$$\begin{aligned} \rho_2(x, t + \tau) = & \int_{-\infty}^{\infty} e^{-k_{21}(t)\tau} \Psi_2(\rho_2(x - z, t)) \rho_2(x - z, t) \Phi_2(z) dz \\ & + (1 - e^{-k_{12}(t)\tau}) \rho_1(x, t) \\ & + e^{-k_{21}(t)\tau} (\rho_2(x, t) - \Psi_2(\rho_2(x, t)) \rho_2(x, t)), \end{aligned} \tag{2}$$

where k_{12} and k_{21} are related to the reaction rates, τ is a characteristic time, $\Phi_{1(2)}(z)$ 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.

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