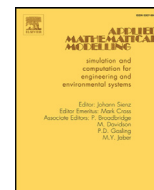




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# A generalized Mittag-Leffler function to describe nonexponential chemical effects

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## ABSTRACT

In this paper a differential equation with noninteger order was used to model an anomalous luminescence decay process. Although this process is in principle an exponential decaying process, recent data indicates that is not the case for longer observation time. The theoretical fractional differential calculus applied in the present work was able to describe this process at short and long time, explaining, in a single equation, both exponential and nonexponential decay process. The exact solution found by fractional model is given by an infinite series, the Mittag-Leffler function, with two adjusting parameters. To further illustrate this nonexponential behavior and the fractional calculus framework, an stochastic analysis is also proposed.

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## 1. Introduction

The question about validation of radioactive decay law has a long history and two reasons for this can be considered. One is that accurate experimental data at very long time are difficult to obtain. For example, for the  $\alpha$ -decay of  $^8\text{Be}$  the deviation from exponential decay is expected after 30 half-lives, when the signal intensity becomes of order  $10^{-7}$  of the initial intensity [1]. The other reason is that the exponential decay law can be derived only as an approximate result of quantum mechanics theory. A rigorous quantum study shows that at very short and very long time unstable state decays with nonexponential dependence of time [2,3].

Until recently the experimental searches for nonexponential behavior was mainly focused on nuclear decay [4–6], in which, as discussed, the experimental measurements are difficult to perform accurately in such a long time. If nonexponential decay is confirmed for nuclear decay, this deviation will affect the radiocarbon dating, as suggested by Aston [7,8]. Experimental effort has now been directed to the study of luminescence decays of some organic materials after pulsed laser excitation [9,10] and in this case the intensity data can be obtained with relatively less difficulty if compared with nuclear radiation decay. The first experimental confirmation of the nonexponential decay law, using luminescence data, was presented by Rothe and coworkers, in 2006 [10]. These authors observed that, as expected, initially luminescence decays obeys the radioactive decay law, but after some half-lives the fluorescence decays significantly slower, turning into a different decaying law. In the study by Rothe and coworkers the experimental data were fitted to two different functions: an exponential function up to about 0.6ns, and after which it was used a power function.

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This problem can be analyzed in different way by using fractional calculus. Recent studies have shown that fractional calculus is a good alternative mathematical tool into many fields of science, such as the study of the growth of bacteria in culture media [11], the mechanisms by which diseases spread [12] and the kinetics of drug absorption [13]. Çalik [14], in which a comparison between experimental data and theoretical model was made with just one half-lives and always at short time when exponential behavior dominates.

In the present work a differential equation with fractional order will be presented as an attempt to generalize the model to exponential and nonexponential luminescence decay of polyfluorene. For the first time, experimental data for luminescence decays, at short and long time, will be compared with the proposed model indicating that fractional model is adequate to describe exponential and nonexponential chemical luminescence decay process. Another issue to be considered here is how to define the probability in this luminescence decay process when described by fractional differential equation. In a comparison with models of integer orders, probability of  $dN$  particles undergoing emission will here be defined using the Mittag-Leffler function.

## 2. Fractional calculus background

Fractional calculus has its roots in a discussion between Leibniz and L'Hospital about the meaning of  $d^{1/2}f(x)/dx^{1/2}$  as described in a book on the subject [15]. Nowadays, fractional calculus is a branch of mathematics analysis that generalizes the derivative and integral with noninteger order.

Theoretical description of fractional calculus may start by integrating  $(Jf)(t) = \int_0^t f(s)ds$  with respect to  $s$  by  $m = (n - l)$  times from which one obtains [15],

$$(J^{(n-l)}f)(t) = \frac{1}{\Gamma(n-l)} \int_0^t (t-s)^{n-l-1} f(s)ds, \quad (1)$$

with  $\Gamma$  the gamma function. On the other hand, the differential operator,  $D$ , can be further applied  $n$  times to this integral to furnish,

$$(D^n J^{n-l} f)(t) = (D^l f)(t). \quad (2)$$

Therefore, for a noninteger number  $l = \alpha$ , one obtains Riemann–Liouville fractional derivative. Another attempt to define was made by Caputo, [15] as:

$$(D^\alpha f)(t) = (J^{n-\alpha} D^n) f(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{f^{(n)}(s)ds}{(t-s)^{\alpha-n+1}}, \quad (3)$$

in which  $n \leq \alpha \leq n + 1$ ,  $\alpha \in \mathcal{R}$ ,  $n \in \mathcal{N}$  and  $f^{(n)}(s) = d^n f/ds^n$ . In this case  $\alpha$  is interpreted as the fractional derivative order. Eq. (3) is known as Caputo fractional derivative of order  $\alpha$ , that is in fact an Abel integral equation [18]. Dealing with fractional derivative and inverting Abel integral equation, an ill-posed problem, are equivalent problems.

The Caputo fractional derivative is a nonlocal operator for it depends on the strain history from 0 to  $t$ . This should be contrasted with a derivative of integer order, a clear local operator. Consequently the fractional derivative in time contains information about the function at earlier points, an effect known as memory effect which will be explored along the current work. This definition to fractional derivative can be used to model the rate change because derivative of a constant is zero, unlike Riemann–Liouville definition. Therefore, henceforth make the assumption that  $D^\alpha f(t)$  is Caputo fractional derivative.

## 3. A generalized decay law

An unimolecular process is described by:

$$dN(t)/dt = -kN(t), \quad (4)$$

with the solution given by  $N(t) = N(0)e^{-kt}$ . The constant  $k$  is the decay constant,  $N(t)$  the number of species present at a time  $t$  and  $N(0)$  is the number of particles at initial time. This is an example of a process described by an integer order derivative. Although the unimolecular model is the one normally used to describe the emission intensity  $I(t) = N(t)/N(0)$  of a luminescence process, recent experimental data evidenciate that cannot be the case for long observation time.

As luminescence decays behavior changes with time, it will be assumed that the memory effect have an important role in decays process. One way to include this effect is to use fractional derivative order in the model. Investigation of the chemical luminescence process by a fractional derivative order has to start by the Caputo derivative,

$$D^\alpha I(t) = -\lambda I(t), \quad (5)$$

and, as to be discussed, will correct to describe luminescence experimental data in both regions: exponential and nonexponential part. This is the first study in the literature of such a data using fractional analysis. If fraction order is equal a one recovers the usual description of this process, Eq. (4). Henceforth we will assume that  $N(0) = 1$  and  $N(t) = I(t)$ .

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