Commun Nonlinear Sci Numer Simulat 25 (2015) 41–49

Contents lists available at ScienceDirect

Commun Nonlinear Sci Numer Simulat

journal homepage: www.elsevier.com/locate/cnsns

Chaos in the fractional order nonlinear Bloch equation with delay

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ARTICLE INFO

Article history:
Received 8 September 2014
Received in revised form 25 November 2014
Accepted 5 January 2015
Available online 19 January 2015

Keywords:
Bloch equation
Fractional calculus
Chaos
Delay
Magnetic resonance
Relaxation

ABSTRACT

The Bloch equation describes the dynamics of nuclear magnetization in the presence of static and time-varying magnetic fields. In this paper we extend a nonlinear model of the Bloch equation to include both fractional derivatives and time delays. The Caputo fractional time derivative (α) in the range from 0.85 to 1.00 is introduced on the left side of the Bloch equation in a commensurate manner in increments of 0.01 to provide an adjustable degree of system memory. Time delays for the z component of magnetization are inserted on the right side of the Bloch equation with values of 0, 10 and 100 ms to balance the fractional derivative with delay terms that also express the history of an earlier state. In the absence of delay, $\tau = 0$, we obtained results consistent with the previously published bifurcation diagram, with two cycles appearing at $\alpha = 0.8548$ with subsequent period doubling that leads to chaos at $\alpha = 0.9436$. A periodic window is observed for the range $0.962 < \alpha < 0.9858$, with chaos arising again as α nears 1.00. The bifurcation diagram for the case with a 10 ms delay is similar: two cycles appear at the value $\alpha = 0.8532$, and the transition from two to four cycles at $\alpha = 0.9259$. With further increases in the fractional order, period doubling continues until at $\alpha = 0.9449$ chaos ensues. In the case of a 100 millisecond delay the transitions from one cycle to two cycles and two cycles to four cycles are observed at $\alpha = 0.8441$, and $\alpha = 0.8635$, respectively. However, the system exhibits chaos at much lower values of α ($\alpha = 0.8635$). A periodic window is observed in the interval $0.897 < \alpha < 0.9341$, with chaos again appearing for larger values of α. In general, as the value of α decreased the system showed transitions from chaos to transient chaos, and then to stability. Delays naturally appear in many NMR systems, and pulse programming allows the user control over the process. By including both the fractional derivative and time delays in the Bloch equation, we have developed a delay-dependent model that predicts instability in this non-linear fractional order system consistent with the experimental observations of spin turbulence.

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http://dx.doi.org/10.1016/j.cnsns.2015.01.004
1007-5704/

1. Introduction

Fractional order derivatives provide a novel approach to modeling the dynamics of complex circuits and systems. In contrast with conventional techniques that introduce complexity in a linear system by increasing the number of components, which increases the order of the system, the 'fractional' approach is to generalize the order of the integer derivatives so that the dynamic behavior will interpolate smoothly between first, second and third order system models [1–6]. Thus, when examining phenomena arising in complex, heterogeneous materials – such as those arising during electrode polarization, viscoelastic creep, or dielectric relaxation – fractional order models are often found to provide a better fit to the experimental data [3–10]. As noted by the mathematician, M. Kac [11], "success is characterized by the fidelity with which such models fit the observed phenomena, and by the sharpness of the questions they pose about the underlying physics." Hence, fractional order models can be viewed as a success because while they sometimes provide improved fits when compared with integer order models, they almost always provoke sharp questions about the underlying conceptual models for the observed phenomena.

This situation has certainly been the case in the application of fractional calculus to problems in nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) [12,13]. NMR and MRI examination of complex, porous and heterogeneous materials (from both living and nonliving systems) yields many opportunities for assessing the ways in which the underlying (sub-voxel) structure influences observed changes in magnetization through the physical processes of relaxation, dispersion and diffusion. Just as a Gaussian distribution follows from assumptions about the statistical behavior of the component particles (e.g., identical and independent events with finite variance) for a random walk (Brownian motion), the Mittag-Leffler function flows from fractional order models that relax the assumptions of independence of earlier times, and exhibit some degree of memory or nonlocal behavior. The utility of fractional order models lies in the adjustable order of the dynamic model.

This paper is part of a series in which we are exploring the utility of generalizing the Bloch equation – which governs the spin dynamics in magnetic resonance imaging (MRI), and magnetic resonance spectroscopy (MRS) – to account for the unexpected experimental observation of spin turbulence (principally the discovery of Huang et al. [14]). Work prior to ours focused on the non-linear, integer order Bloch equation, with and without delay, and this work, unfortunately, was not able to explain all of the observed features of spin turbulence. The issue is critical because, without a full understanding of the conditions governing the onset of such chaotic dynamics, the clinical and experimental use of MRI and MRS could be compromised. Our experience with numerical models of linear and non-linear, fractional order versions of the Bloch equation (with and without delay) [15–17] encouraged us to examine spin turbulence more completely. Physical interest in the fractional order Bloch equation has been growing [12,13] with the goal of improving the modeling of relaxation, diffusion, and perfusion in biological tissues. It is the heterogeneity, porosity, and tortuosity of tissue that instills complexity in the measurements of the relaxation times (T_1, T_{1rho} and T_2), the diffusion coefficient (apparent, anisotropic, and anomalous), and local blood flow (laminar, turbulent, and intravoxel incoherent motion).

The rationale for the work described in this paper is that fractional derivatives may improve our understanding of the dynamic events that occur in biological tissues. Such understanding is fundamental in NMR and MRI where bioengineers and physicians seek to describe the underlying multi-scale processes that occur, for example, when tissues are developing, regenerating, or injured and in need of repair. Fractional order models work well in describing NMR relaxation and diffusion when the governing Bloch equations are linear and the derivatives exhibit no explicit delays [12,13]. However, many problems cannot be completely formulated within this framework, and in such cases, mathematical complexity and chaos can occur [18]. Therefore, to address such phenomena in a systematic way, we have developed new numerical tools. In the past we have applied these tools to examine chaos in the Bloch equation (fractional and integer order) and have sought to understand how delays inherent in the Bloch equation will manifest themselves [15–17]. In this paper we examine the onset of chaos in a specific NMR system in which both fractional order derivatives and delay are present.

2. Background

We are striving in this work to expand the suite of mathematical techniques that can be applied to describe spin turbulence. Since this phenomenon is not yet fully understood, we seek to explore the influence of fractional order operators and delay on the onset of chaos in the governing Bloch equation. NMR, which provides the basis for MRI, is fundamentally described by the Bloch equation: a set of linear, first-order ordinary differential equations [19]. This model is adequate for describing spin polarization, relaxation and diffusion in simple liquids and gels with a relatively homogeneous composition [20].

We have been exploring the utility of generalizing the Bloch equation to fractional order since 2006 in a series of papers [12,13,15–17]. Briefly, we were stimulated to consider fractional order derivatives by the observation that anomalous diffusion, when characterized as a continuous time random walk (CTRW), is the natural solution to a fractional order generalization of the classical diffusion equation expressed as the stretched Mittag-Leffler function [12]. This approach was validated in experimental studies of rat brain structure [21] and extended to analyze distributions of NMR relaxation times in [13] which was applied to the analysis of diffusion in gels [22] and of relaxation in cartilage [23]. The underlying connection between these models and material structure is the appearance of multi-scale, self-similarity in tissue, gels and composites. We