Chapter 8

Fractional Bloch Equation with Delay

This chapter is based on the following paper:
8.1 Introduction

The classical description of nuclear magnetic resonance (NMR) - the phenomena underlying magnetic resonance imaging (MRI) - is summarized in vector form by the Bloch equation [1, 10],

\[
\frac{d \vec{M}}{dt} = \gamma \vec{M} \times \vec{B} - \frac{(M_z - M_0)}{T_1} i_z - \frac{(M_x i_x + M_y i_y)}{T_2},
\]  

(8.1)

where \(\vec{M}(M_x, M_y, M_z)\) represents the time-varying magnetization (Amps/s), \(M_0\) the equilibrium magnetization, \(\vec{B}(B_x, B_y, B_z)\) the applied radiofrequency (RF), gradient and static magnetic fields (Tesla), \(\gamma\) is the gyromagnetic ratio (42.57 MHz/Tesla, for spin 1/2 protons), and \(T_1, T_2\) are the spin-lattice and the spin-spin relaxation times, respectively. For homogeneous (e.g., over a 1-2 mm\(^3\) voxel), and isotropic materials with a single spin component (typically water protons), the Bloch equation prescribes the dynamic balance between externally applied magnetic fields and internal sample relaxation times. This dynamic balance is the basis for pulse sequence design, signal acquisition, image reconstruction and, in the case of MRI, tissue contrast [3, 13, 24].

Fractional order generalization of the Bloch equation has been undertaken by several groups [16, 17, 23] to account for the anomalous relaxation and anomalous diffusion observed in NMR studies of complex materials - typically gels, emulsions, porous composites and biological tissues. A common feature of such complex materials is a “mesoscopic” structure intermediate in scale between the molecular and the macroscopic regimes. NMR spectroscopy and MRI are powerful experimental tools for probing the organization (ordered/disordered) and the dynamics (phase transitions, diffusion, permeability) of mesoscopic structures.

However, the application of these experimental tools and the analysis of the acquired data are highly dependent upon the theoretical assumptions underlying the Bloch equation. To the extent that these assumptions apply to a particular material or to a transition between different material phases, conventional NMR analysis is valid and appropriate. Nevertheless, experimental evidence on complex materials strongly suggests anomalous dynamic behavior. This anomalous behavior appears to reflect distributions of relaxation times, and multi-scale phenomena that in some cases suggest a fractal-like structure, non-
local interactions, fading memory etc. Hence, it is anticipated that NMR and MRI measurements of complex materials will show fractional order dynamic behavior.

In this chapter we investigate the effect of introducing a short time delay into the fractional order model. Such time delays may perhaps be used to capture some of the longer time dynamic changes in complex systems associated with aging in both the experimental and system senses.

8.2 Fractional Bloch equation with delay

We apply the method described in Chapter 7 for solving fractional order Bloch equation involving time delay

\[
T^{-\alpha}D^\alpha M_x(t) = \tilde{\omega}_0 M_y(t - \tau) - \frac{M_x(t - \tau)}{T_2}, \tag{8.2}
\]

\[
T^{-\alpha}D^\alpha M_y(t) = -\tilde{\omega}_0 M_x(t - \tau) - \frac{M_y(t - \tau)}{T_2}, \tag{8.3}
\]

\[
T^{-\alpha}D^\alpha M_z(t) = \frac{M_0 - M_z(t - \tau)}{T_1}, \tag{8.4}
\]

\[
M_x(t) = 0, \quad M_y(t) = 100, \quad M_z(t) = 0, \quad \text{for } t \leq 0, \tag{8.5}
\]

where

\[
\tilde{\omega}_0 = \frac{\omega_0}{T_0^{\alpha - 1}} = (\omega_0 T)T^{-\alpha}, \quad \frac{1}{T_1} = \frac{1}{T_1} = \frac{T}{T_1}T^{-\alpha}, \quad \frac{1}{T_2} = \frac{1}{T_2} = \frac{T}{T_2}T^{-\alpha}. \quad \text{We assume that } T = 1.0. \quad \text{In our case we have}
\]

\[
\tilde{\omega}_0 = 320 \times \pi, \quad T_1' = 1, \quad T_2' = 20 \times 10^{-3}, \quad M_0 = 100. \quad \text{We mention that } \tilde{\omega}_0, \frac{1}{T_1} \text{and } \frac{1}{T_2} \text{have the unit of } (\text{sec})^{-\alpha}.
\]

We use the stability analysis by Deng given in Chapter 6 to study the behavior of the system (8.2)--(8.4). Note that, equation (8.4) can be transformed to

\[
D^\alpha M_{z1}(t) = -M_{z1}(t - \tau), \tag{8.6}
\]

where \(M_{z1}(t) = (M_z(t) - M_0)/T_1\). The characteristic equation for this system becomes:

\[
\left(\lambda^{2\alpha} + \frac{2}{T_2} \lambda^\alpha e^{-\lambda \tau} + \left(\frac{1}{\omega_0^2} + \frac{1}{T_2^2}\right) e^{-2\lambda \tau}\right)\left(\lambda^\alpha + e^{-\lambda \tau}\right) = 0. \tag{8.7}
\]

Note that the factor \(\left(\lambda^{2\alpha} + 100\lambda^\alpha e^{-\lambda \tau} + \left(102400\pi^2 + 2500\right) e^{-2\lambda \tau}\right)\) in (8.7) corresponds to equations (8.2)--(8.3) and the factor \(\left(\lambda^\alpha + e^{-\lambda \tau}\right)\) corresponds to a decoupled equation (8.6). We rename (8.2)--(8.3) as subsystem (A) and (8.6) as subsystem (B).
The system changes its behavior (from damped oscillations to oscillations with an increasing height) for a suitable values of delay. Note that when the delay is zero, the solutions to this system of fractional order differential equations are given in [17]. When $\alpha = 1$ and the delay is zero, we find the classical results.

### 8.3 Results

The observations are summarized in Figures 8.1 through 8.6. We consider three values of $\alpha$ for both system A and system B. In this example we assume a perfect spin excitation ($\frac{\pi}{2}$), so that $M_x(0) = 0, M_y(0) = M_0, M_z(0) = 0$. This system should return to equilibrium at long times compared with $T_1$ and $T_2$, that is $M_x(\infty) = 0, M_y(\infty) = 0, M_z(\infty) = M_0$

In the case of $\alpha = 0.80$

for $\tau = 0.00006$, roots of the characteristic equation (8.7) corresponding to system (A) are $-143.972 \pm 5729.25i$ and corresponding to system (B) are $-163062 \pm 123853i$. In view of the Deng’s analysis given in Chapter 6, the system has stable solutions in this case. The numerical results also have the same conclusions. The damped oscillations of $M_x$ and $M_y$ are shown in Figs. 8.1(a) and 8.1(b), whereas Fig. 8.1(c) shows the stable solution for $M_z$.

When $\tau$ is increased to 0.00007, the roots of characteristic equation become $184.389 \pm 5575.72i$ (system (A)) and $-135039 \pm 9804.27i$ (system (B)). Since the real parts of roots for system (A) are non-negative, we can not use the Deng’s analysis (Chapter 6). The numerical results shows that the system (A) becomes unstable for these values of parameters. In Figs. 8.2(a) and 8.2(b) the oscillations of $M_x$ and $M_y$ are with increasing height. This behavior is not normally observed in NMR experiment without delay unless addition RF pulses are applied that generate so called spin echos. The system (B) is stable (Fig. 8.2(c)) in this case.

In the case of $\alpha = 0.90$

damped oscillations of $M_x$ and $M_y$ are observed for $\tau = 0.00009$ (Figs. 8.3(a), 8.3(b)). This observation by numerical method is supported by the theory also, as the roots of the characteristic equation corresponding to system (A) are $-26.4959 \pm 2175.72i$. Also for system (B), the roots are $-116677 \pm 3817.75i$ and the system is stable (Fig. 8.3(c)).
For $\tau = 0.00010$, the characteristic roots become $23.2458 \pm 2164.4i$ (system (A)) and $-103972 \pm 3439.19i$ (system (B)). The numerical solutions (Figs. 8.4(a), 8.4(b)) shows that the system (A) is unstable and system (B) (Fig. 8.4(c)) is stable.

In the case of $\alpha = 1.00$:

it can be observed from analytically and numerically that the system is stable for $\tau = 0.00004$ (Figs. 8.5(a)–(c)). This is the expected classical behavior. For $\tau = 0.00006$, oscillations of $M_x$, $M_y$ with increasing height are observed (Figs. 8.6(a), 8.6(b)) and $M_z$ is stable (Fig. 8.6(c)).

Thus, even for the integer order time derivative, a short time delay is sufficient to bring about a shift in the dynamical behavior of the system. In addition all three values of $\alpha(0.80, 0.90, 1.0)$ a very short time delay ($\tau = 0.000001sec$) yielded only stable anomalous relaxations via Mittag-Leffler functions. In this example we have assume $\omega_0 = 160 \times 2\pi rad/s$. This corresponds to a sinusoidal oscillator with a period of ($T_0 = \frac{2\pi}{\omega_0}$) of 6.25 msec, while the delay typically range from 40-100 $\mu$sec. No available behavior was observed for delay of 1 $\mu$sec.

Figure 8.1: A set of plots of magnetization versus time for the $M_x$, $M_y$ and $M_z$ relaxation dynamics following a 90x degree pulse excitation (a, b, and c respectively) and a two dimensional plot of $M_x$ versus $M_y$ (d) and a three dimensional plot of $M_x$, $M_y$ and $M_z$ (e).
In this figure the time delay was 0.00006 seconds and the value of $\alpha$ was 0.8.

Figure 8.2: A set of plots of magnetization versus time for the $M_x$, $M_y$ and $M_z$ relaxation dynamics following a 90$\degree$ degree pulse excitation (a, b, and c respectively) and a two dimensional plot of $M_x$ versus $M_y$ (d) and a three dimensional plot of $M_x$, $M_y$ and $M_z$ (e). In this figure the time delay was 0.00007 seconds and the value of $\alpha$ was 0.8.
Figure 8.3: A set of plots of magnetization versus time for the $M_x$, $M_y$ and $M_z$ relaxation dynamics following a 90° degree pulse excitation (a, b, and c respectively) and a two dimensional plot of $M_x$ versus $M_y$ (d) and a three dimensional plot of $M_x$, $M_y$ and $M_z$ (e). In this figure the time delay was 0.00009 seconds and the value of $\alpha$ was 0.9.
Figure 8.4: A set of plots of magnetization versus time for the $M_x$, $M_y$ and $M_z$ relaxation dynamics following a 90x degree pulse excitation (a, b, and c respectively) and a two dimensional plot of $M_x$ versus $M_y$ (d) and a three dimensional plot of $M_x$, $M_y$ and $M_z$ (e). In this figure the time delay was 0.00010 seconds and the value of $\alpha$ was 0.9.
Figure 8.5: A set of plots of magnetization versus time for the $M_x$, $M_y$, and $M_z$ relaxation dynamics following a 90x degree pulse excitation (a, b, and c respectively) and a two dimensional plot of $M_x$ versus $M_y$ (d) and a three dimensional plot of $M_x$, $M_y$ and $M_z$ (e). In this figure the time delay was 0.00004 seconds and the value of $\alpha$ was 1.0.
Figure 8.6: A set of plots of magnetization versus time for the $M_x$, $M_y$ and $M_z$ relaxation dynamics following a 90° degree pulse excitation (a, b, and c respectively) and a two dimensional plot of $M_x$ versus $M_y$ (d) and a three dimensional plot of $M_x$, $M_y$ and $M_z$ (e). In this figure the time delay was 0.00006 seconds and the value of $\alpha$ was 1.0.

### 8.4 Discussion

In this chapter we have investigated a generalization of the Bloch equation that includes both fractional derivatives and time delays. The fractional derivative appears on the left side of the Bloch equation, hence the equation is asymmetric with the memory encoded in the definition of the fractional derivative contributing only to one part of the dynamic model for magnetization. In order to account for this discrepancy, we have introduced system memory on the right side of the Bloch equation through a finite time delay - $\tau$. Therefore, by including both the fractional derivative and finite time delays in the Bloch equation, we believe that we have established a more complete and more realistic model for NMR resonance and relaxation. In the following we will describe more completely our rationale for this generalization and the implications of our results for the analysis of
NMR signals. The application of fractional calculus to NMR is relatively recent and it can be seen in the seminal papers [16, 17, 23] directed toward generalizing the dynamics of signal decay due to diffusion and due to relaxation.

The form of the solutions obtained in this study, of course, converged to the results of this previous work when the delay ($\tau$) is zero as well as the classical solutions to NMR precession and relaxation when the fractional order of the derivative is set to equal one. One aspect of the fractional order model is the interconnection between precession and relaxation that arises due to the fact that, unlike the ordinary exponential, the Mittag-Leffler function can not be simply factored. In fact, this model is very much like that reported in [20, 21] where solutions to the damped fractional oscillator are expressed by them in terms of fractional exponential functions via fractional trigonometry. In the future, experimental NMR work is needed to search for such behavior. Additionally, other fractional order generalizations of the Bloch equation should be explored that do not affect precession. Differential equations with delay, however, have almost as long a history as that of fractional calculus - dating back at least to Laplace and Condorcet in the eighteenth century [8]. Today, differential equations with delay are a mainstay of population biology through the so-called predator-prey equations that predict future population growth based not on current numbers of a given species, but on the population sizes at some time in the past (see, for example Refs. [11, 18]). The solutions to such problems are not easy, even in the simplest cases, as one must specify an initial history function and test for the stability of the solutions [8]. Here we have followed the recent techniques from [8] to solve the fractional order model of the Bloch equation with delay. In our analysis, we distinguished two subsystems (A for $T_2$ relaxation, and B for $T_1$ relaxation). In the case of $T_1$ relaxation, our equation (8.6) is equivalent to equation 10 analyzed in [14] and equation 7 analyzed in [5]. These two groups found that this subsystem is stable when $K_p$ is less than one. Since, our model, $K_p$ is minus one, we anticipate stable behavior and that in fact was what was observed in our numerical examples for delays on the order of 10 to 100 microseconds. For much shorter delays (order of 1 microsecond) both subsystems A and B were stable, and mimicked typical fractional order relaxation expressed through the Mittag-Leffler function (with a complex argument). As the delay increased for subsystem A ($T_2$ relaxation), this initial relaxation response was lost and the system transitioned to an
unstable state with growing oscillations of the transverse magnetization. The exact value depended upon the fractional order. It is, of course, also dependent upon the precessional frequency (160 Hz) and the $T_2$ (20 milliseconds). Applying the stability analysis obtained in [5] gives in all cases a reasonable estimate of this system transition.

The results presented in this chapter demonstrate that solutions to the generalized fractional order Bloch equation with delay exhibit novel behavior dependent upon the selected system parameters. In general, for short delays the system relaxes with fractional order decay. While the $T_1$ relaxation is stable for all values of the chosen delay ($\tau$), $T_2$ relaxation is not and after a critical value of $\tau$ exhibits an unstable and increasing sinusoid oscillation. The emergence of this behavior is consistent with the current stability theory for these systems. The likelihood of such behavior occurring in experimental systems is unknown at present, but possible, as such growing oscillations (spin echoes) are observed in integer order systems following multiple RF excitation pulses. Further work is needed to connect the new fractional order models with delay to the NMR behavior of complex molecules and materials.
Bibliography


