Available online at www.sciencedirect.com
ScienceDirect
Journal of Magnetic Resonance 188 (2007) 330–336
JMR Journal of Magnetic Resonance
www.elsevier.com/locate/jmr

Optimal control design of excitation pulses that accommodate relaxation

Naum I. Gershenzon [a], Kyryl Kobzar [b], Burkhard Luy [b], Steffen J. Glaser [b], Thomas E. Skinner [a,*]

[a] *Physics Department, Wright State University, Dayton, OH 45435, USA*
[b] *Institut für Organische Chemie und Biochemie II, Technische Universität München, Lichtenbergstr. 4, 85747 Garching, Germany*

Received 11 May 2007; revised 23 July 2007
Available online 16 August 2007

Abstract

An optimal control algorithm for mitigating the effects of T_1 and T_2 relaxation during the application of long pulses is derived. The methodology is applied to obtain broadband excitation that is not only tolerant to RF inhomogeneity typical of high resolution probes, but is relatively insensitive to relaxation effects for T_1 and T_2 equal to the pulse length. The utility of designing pulses to produce specific phase in the final magnetization is also presented. The results regarding relaxation and optimized phase are quite general, with many potential applications beyond the specific examples presented here.

Keywords: RC-BEBOP; Relaxation; T_1 relaxation; T_2 relaxation; Optimal control theory

1. Introduction

Optimal control theory has proven to be an extremely flexible and powerful tool for designing pulses for NMR spectroscopy. A particularly challenging problem, that of producing uniform excitation over a broad range of chemical shift offsets and RF field inhomogeneity/miscalibration, simultaneously, has been solved in a series of papers demonstrating Broadband Excitation by Optimized Pulses (BEBOP) [1–5]. The minimum pulse length of a given BEBOP depends upon the performance level required for the specific range of offset and RF variation accommodated [3], but it can significantly exceed the length of a hard pulse that would conventionally be used to excite the same bandwidth (albeit nonuniformly and with poor tolerance to RF inhomogeneity). So far, we have assumed that the longitudinal, T_1, and transverse, T_2, relaxation times are much larger than the duration of the pulse, which will not always be the case in practice. We therefore consider the design of BEBOPs that can minimize relaxation effects, or Relaxation Compensated-BEBOP.

The effect of relaxation on pulse performance has been studied in detail by Hajduk et al. [6]. When T_2 and/or T_1 are comparable to the pulse length, t_p, they not only found the expected loss of signal due to relaxation, but a significant degradation in uniformity of the excitation profile for all the pulses they considered. However, the literature on actual pulse design to mitigate the effects of relaxation appears to be relatively sparse and applied to narrowband, selective pulses. Nuzillard and Freeman modified BURP pulses to obtain more uniform response over the selected bandwidth with SLURP [7], but accepted what might be considered the inevitable attenuation due to short T_1, T_2. Rourke et al. [8] later developed an iterative method for designing selective pulses to compensate for transverse relaxation. The procedure they presented did not accommodate either T_1 effects or RF inhomogeneity. They obtained a significant improvement in the uniformity of pulse response, but actual T_2 losses were not provided, and the method assumes $1/T_2$ is small [9]. Reference [9]

* Corresponding author. Fax: +1 937 775 2222.
E-mail addresses: glaser@ch.tum.de (S.J. Glaser), thomas.skinner@wright.edu (T.E. Skinner).

1090-7807/$ - see front matter © 2007 Elsevier Inc. All rights reserved.
doi:10.1016/j.jmr.2007.08.007

derives a method for inverting the Bloch equation at a single resonance offset for the special case $T_1 = T_2$. Its primary application is to pulses which select a specific relaxation rate, which is different than what we are considering here.

Expanding on these earlier works, we explore more generally the possibilities for reducing relaxation effects during long RF pulses (i.e., relative to T_2 and/or T_1). Optimal control can consider both T_1 and T_2 relaxation together with RF inhomogeneity over any specified range of offsets, either connected or disjoint. Moreover, there is a physical basis for expecting to be able to compensate for relaxation during the pulse: we can (i) use the long duration of the pulse to position spins of different chemical shift at appropriate orientations near the z axis that enable them to be subsequently transformed to the x, y plane by a short pulse segment, reducing net T_2 relaxation during the total pulse and (ii) utilize the moderate, but still significant, repolarization that occurs for short T_1. These possibilities for reducing relaxation effects are found quite naturally by the optimal control algorithm, as shown in what follows. There does not appear to be any other study which attempts to reduce the effects of relaxation in pulses of length similar to T_1, T_2.

2. Theory and methods

Optimal control theory applied to NMR spectroscopy has been described in detail elsewhere [1–5,10–12], for systems with no relaxation (i.e., infinite T_1, T_2). Here we reiterate the main theoretical aspects and introduce the necessary modifications associated with finite T_1, T_2.

During the time interval $[t_0, t_p]$, we seek to transfer initial z magnetization $\boldsymbol{M}(t_0)$ for a system of non-interacting spins to a desired final state $\boldsymbol{F}$ over a given range of chemical shift offsets $\Delta\omega$ and RF field inhomogeneity/miscalibration for specified values of T_1 and T_2. The spin trajectories $\boldsymbol{M}(t)$ are constrained by the Bloch equation

$$\dot{\boldsymbol{M}}(t) = \boldsymbol{\omega}_e(t) \times \boldsymbol{M}(t) + D[\boldsymbol{M}_0 - \boldsymbol{M}(t)], \tag{1}$$

where $\boldsymbol{M}_0 = \hat{z}$ is the unit equilibrium polarization for appropriately normalized units, the effective field, $\boldsymbol{\omega}_e$, in angular frequency units (rad/s) is given in terms of the time-dependent RF amplitude, ω_1, and phase, ϕ, as

$$\begin{aligned}\boldsymbol{\omega}_e(t) &= \omega_1(t)[\cos\phi(t)\ \hat{\boldsymbol{x}} + \sin\phi(t)\ \hat{\boldsymbol{y}}] + \Delta\omega\ \hat{\boldsymbol{z}} \\ &= \boldsymbol{\omega}_{rf}(t) + \Delta\omega\ \hat{\boldsymbol{z}},\end{aligned} \tag{2}$$

and the relaxation matrix is

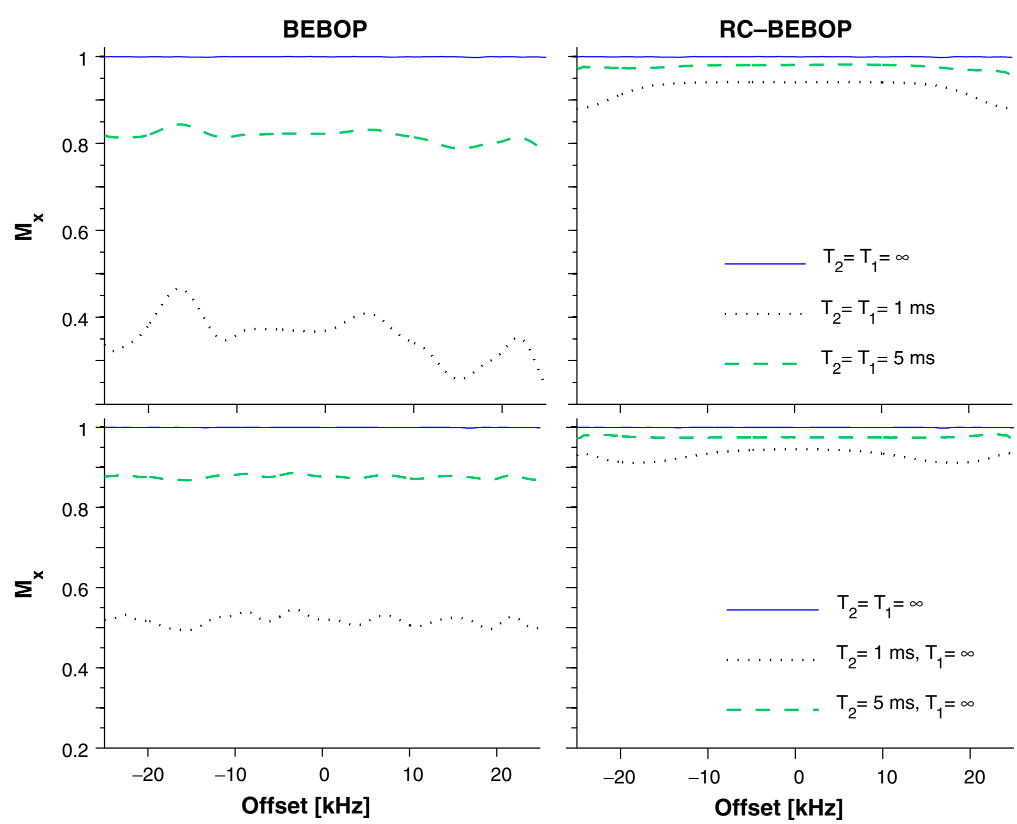

Fig. 1. Simulated performance of the phase-modulated BEBOP from Ref. [5] (left panel) and corresponding relaxation-compenstated RC-BEBOP pulses (right panel) for the T_1 and T_2 values listed on the right. The length of both pulses is 1 ms. The M_x-component of magnetization is plotted as a function of resonance offset, with the nearly perfect performance of the pulses in the absence of relaxation illustrated by the solid blue line at the top of each figure. PM-BEBOP performance is significantly degraded for short T_2 (bottom panels) and short $T_2 = T_1$ (top panels), while RC-BEBOP achieves performance comparable to the case of no relaxation.