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A theoretical and numerical consideration of the longitudinal and transverse relaxations in the rotating frame

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ABSTRACT

We previously derived a simple equation for solving time-dependent Bloch equations by a matrix operation. The purpose of this study was to present a theoretical and numerical consideration of the longitudinal ($R_{1\rho} = 1/T_{1\rho}$) and transverse relaxation rates in the rotating frame ($R_{2\rho} = 1/T_{2\rho}$), based on this method. First, we derived an equation describing the time evolution of the magnetization vector ($\mathbf{M}(t)$) by expanding the matrix exponential into the eigenvalues and the corresponding eigenvectors using diagonalization. Second, we obtained the longitudinal magnetization vector in the rotating frame ($\mathbf{M}_{1\rho}(t)$) by taking the inner product of $\mathbf{M}(t)$ and the eigenvector with the smallest eigenvalue in modulus, and then we obtained the transverse magnetization vector in the rotating frame ($\mathbf{M}_{2\rho}(t)$) by subtracting $\mathbf{M}_{1\rho}(t)$ from $\mathbf{M}(t)$. For comparison, we also computed the spin-locked magnetization vector. We derived the exact solutions for $R_{1\rho}$ and $R_{2\rho}$ from the eigenvalues, and compared them with those obtained numerically from $\mathbf{M}_{1\rho}(t)$ and $\mathbf{M}_{2\rho}(t)$, respectively. There was excellent agreement between them. From the exact solutions for $R_{1\rho}$ and $R_{2\rho}$, $R_{2\rho}$ was found to be given by $R_{2\rho} = (2R_2 + R_1)/2 - R_{1\rho}/2$, where R_1 and R_2 denote the conventional longitudinal and transverse relaxation rates, respectively. We also derived $\mathbf{M}_{1\rho}(t)$ and $\mathbf{M}_{2\rho}(t)$ for bulk water protons, in which the effect of chemical exchange was taken into account using a 2-pool chemical exchange model, and we compared the $R_{1\rho}$ and $R_{2\rho}$ values obtained from the eigenvalues and those obtained numerically from $\mathbf{M}_{1\rho}(t)$ and $\mathbf{M}_{2\rho}(t)$. There was also excellent agreement between them. In conclusion, this study will be useful for better understanding of the longitudinal and transverse relaxations in the rotating frame and for analyzing the contrast mechanisms in $T_{1\rho}$- and $T_{2\rho}$-weighted MRI.

1. Introduction

Recently, the longitudinal and transverse relaxations in the rotating frame have attracted great interest, because they have the potential to provide novel and unique image contrasts that are not available from conventional magnetic resonance imaging (MRI) techniques and they are more sensitive to molecular motion than those obtained by conventional MRI techniques [1].

Michaeli et al. [2] reported that measurements of the longitudinal relaxation time in the rotating frame ($T_{1\rho}$) and transverse relaxation time in the rotating frame ($T_{2\rho}$) provide a possibility to generate MRI contrasts in the human brain, and that their contrasts provide information on different relaxation mechanisms: $T_{1\rho}$ reflects differences in cell density predominantly by its specificity to interactions between water associated with macromolecules and free water, and therefore might provide an indication of neural loss in Parkinson's disease with higher sensitivity than conventional longitudinal relaxation time (T_1); $T_{2\rho}$ is sensitive to diffusion and exchange of water protons in environments with different local magnetic susceptibilities and likely reflects iron content with higher sensitivity than conventional transverse relaxation time (T_2). Nestrasil et al. [3] reported that the shortening of $T_{2\rho}$ is an indicator of iron content in the brain tissue. Micheli et al. [2] also mentioned that $T_{1\rho}$ and $T_{2\rho}$ measurements are complementary to each other, and could be useful for investigating neurodegenerative disorders.

Sierra et al. [4] reported that $T_{1\rho}$- and $T_{2\rho}$-weighted MRI is a useful tool to quantify early changes in water dynamics, reflecting the treatment response during gene therapy. Jokivarsi et al. [5] applied $T_{1\rho}$- and $T_{2\rho}$-weighted MRI to quantitative assessment of water pools in acute cerebral ischemia of the rat, and suggested that physico-chemical models of the rotating frame relaxation may provide insight into the progression of ischemia *in vivo*.

Recently, the chemical exchange saturation transfer (CEST) between solute protons and bulk water protons has also attracted great interest [6,7], because CEST can provide a novel probe to detect dilute proteins/peptides, metabolites, and macromolecules [8–10], as well as their chemical environments [11]. When we consider the

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longitudinal and transverse relaxations in the rotating frame under biological conditions including those pools, it will be essential to take a 2-pool chemical exchange model into account.

Despite much progress in our understanding of the longitudinal relaxation in the rotating frame, theoretical descriptions and applications of the transverse relaxation in the rotating frame have been limited [4].

We previously derived a simple equation for solving the time-dependent Bloch equations using a matrix operation [12], and presented a method for visualizing the trajectory of a magnetization vector in MRI with or without spin lock [13]. The purpose of this study was to present a theoretical and numerical consideration of the longitudinal and transverse relaxations in the rotating frame without and with the CEST effect, by use of these methods [12,13].

2. Materials and methods

2.1. One-pool model

2.1.1. Bloch equations

The time-dependent Bloch equations for constant radiofrequency (RF) irradiation in the absence of diffusion can be given in a rotating frame with the same frequency as that of the RF pulse as follows [12,14]:

$$\begin{cases} \dfrac{dM_x(t)}{dt} = \Delta\omega M_y(t) - R_2 M_x(t) \\ \dfrac{dM_y(t)}{dt} = -\Delta\omega M_x(t) - R_2 M_y(t) + \omega_1 M_z(t) \\ \dfrac{dM_z(t)}{dt} = -\omega_1 M_y(t) - R_1\left[M_z(t) - M_z^0\right] \end{cases} \tag{1}$$

where $M_x(t)$, $M_y(t)$, and $M_z(t)$ denote the x-, y-, and z-components of the magnetization in the rotating frame at time t, respectively, ω_1 the amplitude of the RF-pulse irradiation with a frequency of ω applied along the x-axis of the rotating frame ($=\gamma B_1$, where γ and B_1 are the gyromagnetic ratio and RF power, respectively), and $\Delta\omega$ ($=\omega_0 - \omega$) the offset frequency of the RF-pulse irradiation with respect to the Larmor frequency (ω_0). R_1 and R_2 denote the relaxation rates, i.e., the reciprocals of the longitudinal (T_1) and transverse relaxation times (T_2), respectively. M_z^0 denotes the thermal equilibrium z-magnetization in the absence of RF-pulse irradiation.

The differential equations given by Eq. (1) can be combined into one vector equation [12]:

$$\frac{d\mathbf{M}}{dt} = \mathbf{A}\cdot\mathbf{M}, \tag{2}$$

where

$$\mathbf{M} = \begin{bmatrix} M_x(t) & M_y(t) & M_z(t) & 1 \end{bmatrix}^T \tag{3}$$

and

$$\mathbf{A} = \begin{pmatrix} -R_2 & \Delta\omega & 0 & 0 \\ -\Delta\omega & -R_2 & \omega_1 & 0 \\ 0 & -\omega_1 & -R_1 & R_1 M_z^0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{4}$$

T in Eq. (3) denotes the matrix transpose.

The solution of Eq. (2) can be given by [12]

$$\mathbf{M}(t) = e^{\mathbf{A}t}\mathbf{M}(0), \tag{5}$$

where $\mathbf{M}(0)$ is the matrix of initial values at $t = 0$. $e^{\mathbf{A}t}$ is the matrix exponential, which can be given by (see Appendix A)

$$e^{\mathbf{A}t} = \mathbf{V}\mathrm{diag}\left[e^{\lambda_1 t},\ e^{\lambda_2 t},\ e^{\lambda_3 t},\ e^{\lambda_4 t}\right]\mathbf{V}^{-1}, \tag{6}$$

where $\mathbf{V}$ is the matrix of eigenvectors (eigenmatrix) for $\mathbf{A}$, and λ_1, λ_2, λ_3, and λ_4 are their eigenvalues.

If $M_x(0) = M_y(0) = 0$ and $M_z(0) = 1$ are assumed, i.e., $\mathbf{M}(0) = [0\ 0\ 1\ 1]^T$, the analytical solutions for the eigenvalues and the corresponding eigenvectors can be derived [12,14,15] and are given in Appendix B. As shown in Appendix B, λ_4 is always zero. Except for λ_4, matrix $\mathbf{A}$ has one real eigenvalue and two complex eigenvalues, and the real parts of these eigenvalues are negative. In the following, we assume that the first eigenvalue (λ_1) of matrix $\mathbf{A}$ is much smaller in modulus than the others, i.e., $|\lambda_1| << |\lambda_2| = |\lambda_3|$.

Substituting Eq. (6) into Eq. (5) and using $\lambda_4 = 0$ yield (see Appendix A)

$$\mathbf{M}(t) = \sum_{i=1}^{4} c_i \mathbf{V}_i e^{\lambda_i t} = \sum_{i=1}^{3} c_i \mathbf{V}_i e^{\lambda_i t} + c_4 \mathbf{V}_4, \tag{7}$$

where c_i ($i = 1, 2, 3, 4$) and $\mathbf{V}_i$ ($i = 1, 2, 3, 4$) denote the constant and the ith eigenvector given in Appendices A and B, respectively. Because

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