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General Analytical Solutions of the Bloch Equations

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It has been known since Torrey's paper (*1*) of 1949 on transient nutations that complete analytical solutions to the Bloch equations (*2*) exist, but to date only approximate (*1, 3–5*) or incomplete (*6*) solutions have been presented. Torrey's approach has also been used successfully to derive approximate solutions for the more complex case of two coupled sets of exchanging Bloch equations (*7*). The Bloch equations are used extensively in the analysis and design of NMR experiments, but it is common either to neglect the effects of relaxation during radiofrequency irradiation or to use numerical methods, because of the lack of full solutions. Although numerical methods are adequate for most purposes, there are a number of computationally intensive areas such as the optimization of composite pulses in the presence of relaxation or the simulation of magnetic resonance imaging experiments where the availability of analytical solutions might materially improve the speed of calculations. As there are a number of typographical and other errors in Ref. (*1*), the derivation is given here in full.

The Bloch equations in the rotating frame of reference (*2*) may be written in the form

$$\frac{du}{d\tau} + \beta u + \delta v = 0 \qquad [1]$$

$$\frac{dv}{d\tau} - \delta u + \beta v + M_z = 0 \qquad [2]$$

$$\frac{dM_z}{d\tau} - v + \alpha M_z = \alpha M_0 \qquad [3]$$

by making the substitutions

$$\tau = \omega_1 t, \quad \alpha = \frac{1}{\omega_1 T_1}, \quad \beta = \frac{1}{\omega_1 T_2}, \quad \delta = \frac{\Delta\omega}{\omega_1}, \qquad [4]$$

where $\omega_1 = \gamma B_1$ and $\Delta\omega$ is the offset from resonance in radians per second. Taking the Laplace transforms of Eqs. [1]–[3] gives

$$(p + \beta)\tilde{u} + \delta\tilde{v} = u_0 M_0 \qquad [5]$$

$$-\delta\tilde{u} + (p + \beta)\tilde{v} + \tilde{M}_z = v_0 M_0 \qquad [6]$$

$$-\tilde{v} + (p + \alpha)\tilde{M}_z = \alpha M_0/p + m_0 M_0, \qquad [7]$$

where $u_0 M_0$, $v_0 M_0$, and $m_0 M_0$ are the initial values of u, v, and M_z. Solving for $\tilde{u}$, $\tilde{v}$, and $\tilde{M}_z$ gives

$$p\Delta(p)\tilde{u}/M_0 = u_0 p[1 + (p + \alpha)(p + \beta)] + \delta\alpha + \delta m_0 p - p\delta v_0(p + \alpha) \qquad [8]$$

$$p\Delta(p)\tilde{v}/M_0 = v_0 p(p + \alpha)(p + \beta) - (\alpha + m_0 p)(p + \beta) + p\delta u_0(p + \alpha) \qquad [9]$$

$$p\Delta(p)\tilde{M}_z/M_0 = (\alpha + m_0 p)[(p + \beta)^2 + \delta^2] + p v_0(p + \beta) + p\delta u_0, \qquad [10]$$

where $\Delta(p)$ is the determinant of the matrix of coefficients in Eqs. [5]–[7]:

$$\Delta(p) = (p + \alpha)(p + \beta)^2 + (p + \beta) + \delta^2(p + \alpha). \qquad [11]$$

This can be factored into the form

$$\Delta(p) = (p + a)[(p + b)^2 + s^2] \qquad [12]$$

with roots $-a$, $-b - is$, and $-b + is$. Analytical expressions for these roots have been given by Hore and McLauchlan (*6*) and may be summarized in the form

$$a = \frac{1}{3}(\alpha + 2\beta) - (\epsilon_+ + \epsilon_-) \qquad [13]$$

$$b = \frac{1}{3}(\alpha + 2\beta) + \frac{1}{2}(\epsilon_+ + \epsilon_-) \qquad [14]$$

$$s = \frac{\sqrt{3}}{2}(\epsilon_+ - \epsilon_-), \qquad [15]$$

where

$$\epsilon_\pm = \sqrt[3]{\frac{\zeta \pm \sqrt{\zeta^2 + 4\eta^3}}{54}} \qquad [16]$$

$$\zeta = \theta(9 - 2\theta^2 - 18\delta^2) \qquad [17]$$

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and

$$\eta = 3(1 + \delta^2) - \theta^2 \quad [18]$$

with $\theta = \alpha - \beta$.

When $(\zeta^2 + 4\eta^3) > 0$, the combined effects of offset from resonance and radiofrequency field strength overcome relaxation, and oscillatory solutions result; when $(\zeta^2 + 4\eta^3) < 0$, relaxation dominates and the system is overdamped. In the latter case, s becomes imaginary and Eq. [11] has three real solutions, giving a triexponential approach to equilibrium.

The transforms $\tilde{u}$, $\tilde{v}$, and $\tilde{M}_z$ can all be expressed in the form

$$\tilde{w}(p) = \frac{g(p)}{p\Delta(p)}, \quad [19]$$

where each has a different polynomial $g(p)$. The three expressions can be expanded in partial fractions to give

$$\tilde{w}(p) = \frac{A}{(p+a)} + \frac{B(p+b)+C}{(p+b)^2+s^2} + \frac{D}{p}, \quad [20]$$

where A, B, C, and D are constants which are functions of α, β, u_0, v_0, etc., and which are different for $\tilde{w} = \tilde{u}$, $\tilde{v}$, and $\tilde{M}_z$, respectively. The inverse Laplace transform of [20] then gives the general form of the solutions for u, v, and M_z,

$$w(\tau) = M_0\left[Ae^{-a\tau} + Be^{-b\tau}\cos s\tau + \frac{C}{s}e^{-b\tau}\sin s\tau + D\right], \quad [21]$$

where the three coefficients D for u, v, and M_z represent the steady-state solutions. In the overdamped case this can also be written as

$$w(\tau) = M_0\left[Ae^{-a\tau} + \left(\frac{B\sigma - C}{2\sigma}\right)e^{-(b+\sigma)\tau} + \left(\frac{B\sigma + C}{2\sigma}\right)e^{-(b-\sigma)\tau} + D\right], \quad [22]$$

where $\sigma = -is$.

Coefficients A and D can be found from

$$D = \lim_{p\to 0}[p\tilde{w}(p)] \quad [23]$$

and

$$A = \lim_{p\to -a}[(p+a)\tilde{w}(p)], \quad [24]$$

giving

$$D = \frac{g(0)}{a(b^2+s^2)} \quad [25]$$

and

$$A = \frac{-g(-a)}{a\{(b-a)^2+s^2\}}, \quad [26]$$

where the polynomials $g(p)$ are

$$g_u(p) = u_0p\{1 + (p+\alpha)(p+\beta)\} + \delta\alpha + \delta m_0 p - p\delta v_0(p+\alpha) \quad [27]$$

$$g_v(p) = u_0\delta p(p+\alpha) + v_0p(p+\alpha)(p+\beta) - (\alpha + m_0p)(p+\beta) \quad [28]$$

$$g_{M_z}(p) = u_0\delta p + v_0p(p+\beta) + (\alpha + m_0p)\{(p+\beta)^2 + \delta^2\}. \quad [29]$$

The constants B and C can be found from the initial values and initial derivatives of u, v, and M_z:

$$w(0) = A + B + D, \quad \frac{dw(0)}{d\tau} = -aA - bB + C. \quad [30]$$

Expanding $\Delta(p)$ in terms of its roots and of α, β, etc., and then equating coefficients give

$$2\beta + \alpha = 2b + a \quad [31]$$

$$2\alpha\beta + \beta^2 + \delta^2 + 1 = 2ab + b^2 + s^2 \quad [32]$$

$$\alpha\beta^2 + \alpha\delta^2 + \beta = ab^2 + as^2. \quad [33]$$

This simplifies [18] to give

$$D_u = \frac{\delta\alpha}{\alpha(\beta^2+\delta^2)+\beta} \quad [34]$$

$$D_v = \frac{-\alpha\beta}{\alpha(\beta^2+\delta^2)+\beta} \quad [35]$$

$$D_{M_z} = \frac{\alpha(\delta^2+\beta^2)}{\alpha(\beta^2+\delta^2)+\beta}, \quad [36]$$

in agreement with the well-known steady-state solutions of the Bloch equations (*2*).

A, B, and C require the roots of $\Delta(p)$. Substitution of Eqs. [27] to [29] into [26] gives

$$A_u = \frac{au_0\{1 + (\alpha - a)(\beta - a)\} - \delta\alpha(1 + v_0 a) + \delta a(m_0 + av_0)}{\gamma} \quad [37]$$

$$A_v = \frac{au_0\delta(\alpha - a) + av_0(\alpha - a)(\beta - a) - (m_0 a - \alpha)(\beta - a)}{\gamma} \quad [38]$$

$$A_{M_z} = \frac{au_0\delta + av_0(\beta - a) - (m_0 a - \alpha) \times \{(\beta - a)^2 + \delta^2\}}{\gamma}, \quad [39]$$

where $\gamma = a\{(b - a)^2 + s^2\}$. From the initial values $w(0)$ [30],

$$B_u = u_0 - (A_u + D_u) \quad [40]$$

$$B_v = v_0 - (A_v + D_v) \quad [41]$$

$$B_{M_z} = m_0 - (A_{M_z} + D_{M_z}), \quad [42]$$

and from the initial values $dw(0)/d\tau$ [30],

$$C_u = aA_u + bB_u - (\beta u_0 + \delta v_0) \quad [43]$$

$$C_v = aA_v + bB_v + \delta u_0 - m_0 - \beta v_0 \quad [44]$$

$$C_{M_z} = aA_{M_z} + bB_{M_z} + v_0 + \alpha(1 - m_0). \quad [45]$$

Substituting the roots of $\Delta(p)$ [13] to [15] and results [34] to [45] into Eq. [21] or [22] then gives the full transient analytical solutions for $u(\tau)$, $v(\tau)$, and $M_z(\tau)$.

Although the analytical expressions found by combining Eqs. [13] to [18], [21], and [34] to [45] are a little unwieldy, they should require significantly less computation than numerical solution of the Bloch equations and should be of use in simulations of spin system response during experiments which involve relaxation during pulses. The analytical results could also be combined with numerical integration methods where slow-exchange processes are present, as, for example, in the simulation of magnetization-transfer contrast experiments in magnetic resonance imaging (*7*).

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