SHAPES OF NUCLEAR INDUCTION SIGNALS UNDER INHOMOGENEOUS MAGNETIC FIELDS

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INTRODUCTION

The shape of the nuclear induction signal is determined by structural types and dynamic processes in the analizable substance. It depends on the conditions of observation: temperature, a radio-frequency (RF) impulse sequence type, a spatial inhomogeneity of the RF field and so on [1, 2]. The magnetic polarizing field inhomogeneity exerts essential influence on nuclear induction signal parameters. The form and the orientation of the sample have also effect. F. Bloch equations describing the motion of the macroscopic nuclear magnetization vector have been solved in case of the homogeneous magnetic field. The inhomogeneity influence is taken into account under the assumption that the real distribution of the magnetic field is known [3 – 5].

SHAPES OF NUCLEAR INDUCTION SIGNALS

In the inhomogeneous magnetic field B_0 ($\vec{B}_0$ is axial $\vec{z}$) and the absence of the electromagnetic field ($\vec{B}_1 = 0$) the x-component (M_x) of the macroscopic nuclear magnetization vector $\vec{M}$ is

$$M_x(t) = M_x(0)\exp(-t/T_2)\cos(\omega_0 t), \tag{1}$$

where $M_x(0)$ – initial value of the transversal component of the magnetization vector, $\omega_0 = \gamma B_0$ the resonant value of the nuclear frequency in the field B_0, γ - gyromagnetic ratio, T_2 – the transverse relaxation time of nuclear spins.

The sample is divided into elementary volumes. The field inside of them is considered to be homogeneous. The signal from the elementary volume is a two-variable function: of time t and of $\Delta\omega_0 = \gamma\Delta B_0$ - a frequency deviation of a nuclear precession from its average value $\omega_0 = \gamma B_0$, where ΔB - induction deviation from its average value B_0 inside the volume element (the spot). In that case

$$M_x(t,\alpha) = M_x(0)\exp(-t/T_2)\cos(\omega^{\bullet} t), \tag{2}$$

here

$$\omega^{\bullet} = (1-\sigma)\omega == (1-\sigma)(\omega_0 + \Delta\omega) =$$
$$= (1-\sigma)(\omega_0 + \alpha) = \gamma(1-\sigma)(B_0 + \Delta B)$$

– a precessional frequency in the elementary volume taking into account the screening magnetic effect, σ - constant of the magnetic screening, α = Δω. Since field deviations from the average value B_0 are small value M(0) – a weak dependence function from inhomogeneity. This dependence is neglected.

The total precession signal from the simple is

$$F_x(t) = \int_{-\infty}^{+\infty} f(\alpha) M_x(t,\alpha)\, d\alpha = \\ = M_x(0)\exp(-t/T_2)\int_{-\infty}^{+\infty} f(\alpha)\cos\omega^*(\alpha) t\, d\alpha \tag{3}$$

In case of the exponential distribution

$$f(\alpha) = \frac{1}{2\beta}\cdot\exp(-|\alpha|/\beta) \tag{4}$$

the total signal with the initial amplitude normalized to unity is

$$F_N(t) = \frac{M_x(t)}{M_x(0)} = \frac{\exp(-t/T_2)}{\sqrt{1+(\beta^* t)^2}}\cdot\cos(\omega_0^* t + \phi), \tag{5}$$

where $\phi = arctg\,(\beta^* t)$, $\beta^* = (1-\sigma)\beta$, $\omega_0^* = (1-\sigma)\omega_0$, this and below index “x” is omitted. The phase of the induction signal is time-depended. Therefore the frequency of total precession signal is changing.

Selecting the field triangular distribution

$$f(\alpha) = \begin{cases} h(1+h\alpha) & by\quad -1/h < \alpha < 0 \\ h(1-h\alpha) & by\quad 1/h > \alpha > 0 \\ 0 & by\quad |\alpha| > 1/h \end{cases}, \quad h > 0$$

it is getting

$$F_N(t) = \left[\frac{\sin(h^* t)}{(h^* t)}\right]^2 \exp(-t/T_2)\cos(\omega_0^* t), \tag{6}$$

where $h^* = (1-\sigma)/2h$.

In case the Lorentz, the Gaussian, the triangular, the impulse (rectangular) field distributions the frequency is $\omega_0^* = const$. Amplitude expressions for the Lorentz, the Gaussian and impulse distributions published in [5] agree with those which we deduced in special case of $\sigma = 0$.

Let’s examine the pulse distribution with finite acceleration time. If the leading edge curve changes by Lorentz law

$$f(\alpha) = \begin{cases} \dfrac{1}{pa} & by\quad |\alpha| \le \dfrac{a}{2} \\ \dfrac{(p-1)T_2'}{p\pi\{1+[(|\alpha| - \frac{a}{2})T_2']^2\}} & by\quad |\alpha| > \dfrac{a}{2} \end{cases},$$

$p \ge 1$

the nuclear induction signal is

$$F_N(t) = A\exp(-t/T_2)\cos(\omega_0^* t + \phi), \tag{7}$$

where

$$A = \frac{1}{p}\sqrt{B(B+C) + (p-1)^2 D},$$

$B = \frac{\sin(a^* t)}{a^* t}$,

$C = 2(p-1)\sqrt{D}\cos(a^* t + \theta)$,

$D = \exp(-2t/T_2^*) + G_M^2/\pi$,

G_M - Meijer G-function of the kind

$MeijerG\ [\{\{\frac{1}{2}\},\{\}\},\{\{\frac{1}{2},\frac{1}{2}\},\{0\}\},\left(\frac{t}{2T_2^*}\right)^2]sign\left[\frac{t}{T_2^*}\right]$,

$\theta = arctg\left\{\frac{G_M \exp(t/T_2^*)}{\pi}\right\}$,

$\phi = arctg\left[\frac{2(p-1)D\sin(a^* t + \theta)}{2B + C}\right]$,

$a^* = (1-\sigma)a/2$, $1/T_2^* = (1-\sigma)/T_2^{'}$.

For a continuously curve it needs $p = 1 + \pi/(aT_2^*)$.

If pulse "wings" modify by Gaussian law

$$f(\alpha) = \begin{cases} \frac{1}{pa} & by\ |a| \le a/2 \\ \frac{p-1}{p\sigma_1\sqrt{2\pi}}\exp\left(\frac{(|\alpha| - a/2)^2}{2\sigma_1^2}\right) & by\ |a| > a/2 \end{cases},$$

$p \ge 1$

the nuclear induction signal is

$$F_N(t) = A\exp(-t/T_2)\cos(\omega_0^* t + \phi), \quad (8)$$

where

$A = \frac{1}{pa^* t}\sqrt{B^2 + \sqrt{1 + (2B)^2}\sin a^* t\cos(a^* t - \theta_1)}$,

$B = (p-1)a^* t\exp(-(\sigma_1^* t)^2)$,

$\theta_1 = arctg\left[\frac{\exp(\sigma_1^* t)^2}{2(p-1)a^* t}\right]$,

$\phi = arctg\left[\frac{B\sin(a^* t)}{\cos(a^* t - \theta_2)\cdot\sqrt{1 + B^2}}\right]$,

$\theta_2 = arctg\left[\left(\frac{\exp((\sigma_1^* t)^2)}{(p-1)a^* t}\right)\right]$,

$\sigma_1^* = \sqrt{2}(1-\sigma)\sigma_1$, $a^* = (1-\sigma)a/2$.

There are not ruptures of the function if

$p = 1 + \sqrt{\pi}\sigma_1^*/a$.

If leading edges modify by exponential law

$$f(\alpha) = \begin{cases} \frac{1}{pa} & by\ |\alpha| \le \frac{a}{2} \\ \frac{p-1}{2\beta p}\exp\left(\frac{\||\alpha| - a/2|}{\beta}\right) & by\ |\alpha| \ge \frac{a}{2} \end{cases}$$

$p \ge 1$

the formula is given by

$$F_N(t) = A\exp(-t/T_2)\cos(\omega_0^* t + \phi), \quad (9)$$

where

$A = \frac{1}{p}\sqrt{[B + C\cos(a^* t + \theta_1)]^2 + [C\cos(a^* t - \theta_2)]^2}$,

$B = (\sin\ a^* t)/(a^* t)$, $C = (p-1)/\sqrt{1 + (\beta^* t)^2}$,

$\theta_1 = arctg\ (\beta^* t)$, $\theta_2 = arctg\ (1/\beta^* t)$,

$\phi = arctg\left[\frac{C\cos(a^* t - \theta_2)}{B + C\cos(a^* t + \theta_1)}\right]$.

There are not jumps of the function if

$p = 1 + (2\beta\exp(\||\alpha| - a/2|)/\beta)/a$.

If leading edges modify by the linear law (the trapezoidal distribution)

$$f(\alpha) = \begin{cases} f_1(\alpha) & by\ -1/h - a/2 < \alpha < -a/2 \\ f_2(\alpha) & by\ |\alpha| \le a/2 \\ f_3(\alpha) & by\ 1/h + a/2 > \alpha > a/2 \\ f_4(\alpha) & by\ |\alpha| > 1/h + a/2 \end{cases}$$

where

$f_1(\alpha) = [(p-1)(h + h^2(\alpha + a/2))]/p$,

$f_2(\alpha) = 1/pa$,

$f_3(\alpha) = [(p-1)[h - h^2(\alpha - a/2)]/p$,

$f_4(\alpha) = 0$,

$p \ge 1$

the expression is given by

$$F_N(t) = (A + B)\exp(-t/T_2)\cos\omega_0^* t. \quad (10)$$

At this point

$A = \frac{1}{p}[\frac{\sin(a^* t)}{a^* t} + \frac{p-1}{2(h^* t)^2}\sqrt{1 + (a^* t)^2}\cos(a^* t - \theta_1)]$,

$B = \frac{p-1}{p}\{\frac{C\sin(h^* t)}{(h^*)^2 t}\cos[(C - h^*)t] - \frac{1}{2(h^* t)^2}\sqrt{1 + (Ct)^2}\cos(Ct - \theta_2)\}$,

$h^* = (1-\sigma)/(2h)$, $C = a^* + 2h^*$, $\theta_1 = arctg(a^* t)$,

$\theta_2 = arctg\ (Ct)$.

Let's consider two sites system (a and b) of the same nuclear spins with a chemical shift $\Delta\omega_{ab} \ne 0$. We will consider fast exchange between components a and b. In this case [6] $C_a, C_b >> 1/T_{2a}, 1/T_{2b}$, $|\omega_a - \omega_b|$ and $(\omega_a - \omega_b)^2 >> (1/T_{2a} - 1/T_{2b})$ the nuclear magnetization is

$M_x = M'(0)\exp(-t/T_2)\sin\omega_{av} t$,

where $M'(0) = k_1 M(0)$, $k_1 \le 1$, $\omega_{av} = P_a\omega_a + P_b\omega_b$,

$\frac{1}{T_{2a}} = \frac{P_a}{T_{2a}} + \frac{P_b}{T_{2b}} + \frac{[1 - (P_b - P_a)^2](\omega_a - \omega_b)^2}{4(C_a + C_b)}$.

Then an average frequency with a gradient is

$\overline{\omega_{abG}^c} = P_a\omega_{aG}^c + P_b\omega_{bG}^c = m(\omega_0 + \alpha)$,

where $m = P_a(1 - \sigma_a) + P_b(1 - \sigma_b)$.

1. For the Gaussian distribution of the field

$f(\alpha) = \frac{1}{\sigma_1\sqrt{2\pi}}\cdot\exp(-\alpha^2/2\sigma_1^2)$

the signal is

$$F_N(t) = A\exp(-Bt - Ct^2)\sin(D\omega_0 t), \quad (11)$$

here

$A = \frac{1}{\sigma_1\sqrt{2d}}$, $B = n + k\omega_0^2$, $C = \frac{m^2 - 4k^2\omega_0^2}{4d}$,

$D = \left(1 - \frac{kt}{d}\right)m$, $d = \frac{1}{2\sigma_1^2} + kt$, $n = \frac{P_a}{T_{2a}} + \frac{P_b}{T_{2b}}$,

$k = \frac{1 - (P_b - P_a)^2}{4(C_a + C_b)}(\sigma_b - \sigma_a)^2$.

2. For the exponential distribution (4) the formula is

$$F_N(t) = A\exp(-nt)\sin(m\omega_0 t), \quad (12)$$

where

$$A = \frac{\left(\frac{1}{\beta} + 2k\omega_0 t\right)\left[\sqrt{\pi}\exp\left(-\frac{m^2}{4k}t\right) + 2\sqrt{kt}\right]}{2\beta\left[\left(\frac{1}{\beta} + 2k\omega_0 t\right)^2 + (mt)^2\right]\sqrt{kt}},$$

n, m, k are the similar as above.

Similar expressions have a place for the component of the longitudinal magnetization $M_z(t)$, if in foregoing formulas $M_x(t,\alpha)$ is replaced by $[M_z^0 - M_z(t,\alpha)]$ and $F_N(t)$ is replaced by $F(t)/[M_z^0 - M_z(0)]$, where M_z^0, $M_z(0) = M_z(t=0)$ - equlibrium and initial values of the longitudinal magnetization M_z.

Now work out the shape of the nuclear induction signal from the cylinder sample under the field with the constant gradient G. Let the gradient is directed along the coil axis coinciding with (B=B$_0$ – Gx). If the coil has got radius r$_0$, the amount of turns N uniformly distributing among the length l the electromotive force (emf) induced in the coil is

$$E(t) = E(0)\frac{e^{-t/T_2}}{2\delta^*\omega_0^* t}\{\frac{2}{T_2}\sin(\delta^* t)\cos[(\omega_0^* - \delta^*)t] +$$
$$+ (\omega_0^* - 2\delta^*)\cos[(\omega_0^* - 2\delta^*)t] - \omega_0^*\cos(\omega_0^* t) + \quad (13)$$
$$+ \frac{2}{t}\sin(\delta^* t)\cos[(\omega_0^* - \delta^*)t]\}$$

where the precession initial amplitude is

$$E(0) = \frac{4\pi}{c}NM(0)\omega_0^* S = \frac{4\pi^2}{c}NM(0)\omega_0^* r_0^2,$$

the cross-section area (circle) is $S = \pi r_0^2$ and

$$\delta^* = \frac{1}{2}\gamma(1-\sigma)Gl.$$

In case $\omega_0^* >> \delta^*$

$$E(t) = E(0)e^{-t/T_2}\frac{\sin(\delta^* t)}{\delta^* t}\{\frac{\cos\omega_0^* t}{\omega_0^* T_2} + \quad (14)$$
$$+ \frac{\sqrt{1+(\omega_0^* t)^2}}{\omega_0^* t}\cos(\omega_0^* t - \theta)\}$$

In extreme case $\omega_0^* >> \delta^*$ and $\omega_0^* T_2 >> 1$

$$E(t) = E(0)\frac{\sqrt{1+(\omega_0^* t)^2}}{\omega_0^* t}\frac{\sin(\delta^* t)}{\delta^* t}\cos(\omega_0^* t - \theta), \quad (15)$$

where $\theta = arctg(\omega_0^* t)$.

If $\omega_0^* t >> 1$ the second factor $\frac{\sqrt{1+(\omega_0^* t)^2}}{\omega_0^* t} \cong 1$ and

$$E(t) = E(0)\frac{\sin(\delta^* t)}{\delta^* t}\sin\omega_0^* t, \quad (16)$$

because $\theta \to \frac{\pi}{2}$ at $\omega_0^* t \to \infty$.

If the field gradient direction is perpendicular to the coil axis (B=B$_0$ – Gz or B=B$_0$ – Gy) the emf value induced in the coil is

$$E(t) = A\exp(-t/T_2)\cos(\omega_0^* t - \psi), \quad (17)$$

where

$$A = 2E(0)\sqrt{B^2 + \left[kr_0 C + \frac{B}{\omega_0^* T_2}\right]^2},$$

$$B = \frac{J_1(\vartheta t)}{\vartheta t}, \quad C = \frac{J_2(\vartheta t)}{\vartheta t}.$$

Here $J_1(\vartheta^* t)$ - Bessel's function of the first order of the first kind, $J_2(\vartheta^* t)$ - Bessel's function of the second order of the first kind, $\vartheta^* = \gamma G^* r_0$, $k = G/B_0$,

$$\psi = arctg\left(\frac{B}{kr_0 C + B/\omega_0^* T_2}\right).$$

At $\omega_0^* T_2 >> 1$

$$E(t) = A_1\exp\left(-\frac{t}{T_2}\right)\cos(\omega_0^* t - \psi_1), \quad (18)$$

$$A_1 = 2E(0)\sqrt{B^2 + [kr_0 C]^2},$$

$$\psi_1 = arctg\left(\frac{B}{kr_0 C}\right).$$

In the limit case $\omega_0^* T_2 >> 1$ and $kr_0 << 1$

$$E(t) = 2E(0)\frac{J_1(\vartheta t)}{\vartheta t}\exp\left(-\frac{t}{T_2}\right)\sin\omega_0^* t, \quad (19)$$

because $\psi_1 \to \frac{\pi}{2}$ at $\frac{J_1(\vartheta t)}{kr_0 J_2(\vartheta t)} \to \infty$.

CONCLUSIONS

The shapes of the nuclear induction signals depend on the inhomogeneity type of the magnetic polarizing field. It is possible to perform effective filtrating of the magnetic resonance signals by the deduced expressions. It enables to increase a precision of the data processing and decrease experimental time.

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