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Communication

Active compensation of rf-pulse transients

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ABSTRACT

A new approach to compensate rf-pulse transients is proposed. Based on the idea of the response theory of a linear system, a formula is derived to obtain the required excitation voltage profile back from the intended target rf-pulse shape. The validity of the formula is experimentally confirmed by monitoring the rf-field created inside the sample coil with a pickup coil. Since this approach realizes accurate rf-pulse shapes without reducing the *Q*-factor of the tank circuit of the probe, it can be used not only to suppress the transient tail of the rf-pulse, but also as a general concept for accurate rf-pulsing.

In the conventional NMR experiments using a tuned resonant circuit, the rf-pulse shape, i.e., the amplitude profile of an oscillating magnetic field created inside the sample coil, deviates from that of the excitation voltage programmed in the NMR spectrometer as the quality factor Q of the probe tank circuit is increased and as the resonance frequency is decreased. In particular, the transient tail of rf pulses has been of considerable concern, because it sets a limit on the minimum receiver dead time before signal acquisition. So far, all previous approaches to shorten the probe recovery time rely upon actively damping the Q factor of the rf-tank circuit [1–6]. In this work, we propose a different solution to this challenge by focusing on the causal relationship between the voltage profile of the rf-pulse programmed in the NMR transmitter and the resultant profile of the rf-field produced inside the NMR coil, and present a procedure for calculating the excitation voltage profile *back from* an arbitrary target rf-pulse shape. This perceptual change, described schematically in Fig. 1, enables us to actively suppress transients and create rf pulses exactly as intended with neither Q-damping nor any modification to the probe circuit. Thus, this approach can be used not only as another method for probe ringing suppression, but also as a general concept of accurate pulsing without Q-damping. In this sense, this work provides an extended idea of dead time reduction by the quench pulse technique used in pulsed ESR experiments [7–9].

In the conventional pulsed NMR, rf-irradiation is applied to a nuclear spin system by transmitting a voltage signal

$$V(t) = a(t)\cos(\omega_0 t + \phi) \tag{1}$$

to a resonant circuit of the probe, and, as a consequence, the nuclear spins in the sample placed inside the NMR coil are exposed to an rf field

$$B_1(t) = b(t)\cos(\omega_0 t + \phi + \phi'). \tag{2}$$

Here, ω_0 represents the resonance frequency of the circuit tuned at the Larmor frequency of the nuclear spins, ϕ is the phase of the rf-irradiation, and ϕ' is a phase offset which depends on the length of the transmission line and passive components such as rf filters. We assume that the envelopes $a(t)$ and $b(t)$ vary slowly in time compared to the period $2\pi/\omega_0$ of the carrier wave. This approximation, known as the Slowly Varying Envelope Approximation (SVEA) and is often treated in laser optics, describes a common situation of NMR experiments in which the Fourier components of a pulse-modulated rf-irradiation lie inside the Q dip of the resonant circuit of the probe.

For a linear system like a resonant circuit used in an NMR probe, the rf-field profile $b(t)$ induced inside the NMR sample coil is represented as

$$b(t) = \int_{-\infty}^{\infty} dt' h(t-t')a(t) = h(t) * a(t), \tag{3}$$

where $h(t)$, known as an impulse response, is the rf-field profile created by a unit impulse excitation. Our interest here is to solve Eq. (3) in terms of the excitation voltage profile $a(t)$ that results in an arbitrary target field profile $b(t)$. Laplace transformation is a powerful mathematical tool for this purpose, since the Laplace transformation of a convolution is equal to the product of the individual Laplace-transformed functions. That is, Eq. (3) is transformed into

$$B(s) = H(s)A(s), \tag{4}$$

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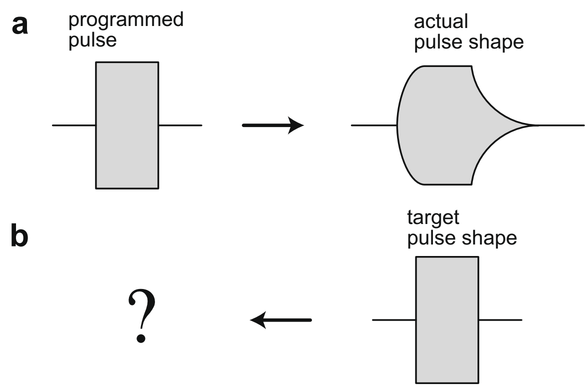

Fig. 1. (a) The rf-pulse shape that the nuclear spins in a tuned coil 'feel' differs from that programmed in the transmitter. The central issue of this work is to provide a procedure for programming the amplitude profile that gives an arbitrary pulse shape of the rf-field inside the coil, as described in (b).

where $B(s) = \int_0^\infty dt e^{-st} b(t), H(s) = \int_0^\infty dt e^{-st} h(t)$, and $A(s) = \int_0^\infty dt e^{-st} a(t)$.

From Eq. (4) we obtain

$$A(s) = \frac{B(s)}{H(s)}. \tag{5}$$

Thus, given the impulse response $h(t)$ of the probe circuit under interest, the rhs of Eq. (5) can be calculated straightforwardly, and its inverse Laplace transformation gives the voltage profile $a(t)$ of the excitation pulse for the target rf-pulse shape $b(t)$ that the nuclear spins inside the coil feel.

We now need the impulse response $h(t)$, which can in principle be derived from the circuit diagram of the probe using the Kirchhoff's law. However, such a case-by-case analysis, albeit rigorous, is somewhat complicated and may not be useful in practice. Here, we resort to a simple approximation of the impulse response by an exponential function, assuming that its time constant τ is given by the relaxation time of the tuned circuit, i.e., $\tau = 2Q/\omega_0$. Then,

$$h(t) = C\exp(-t/\tau) = C\exp\left[-\frac{\omega_0 t}{2Q}\right], \tag{6}$$

where C is a constant having a dimension of T V^{-1} s^{-1} and depends on the hardware in use. By Laplace-transforming Eq. (6), we obtain

$$H(s) = \frac{C}{s + 1/\tau}, \tag{7}$$

and hence

$$CA(s) = (s + 1/\tau)B(s). \tag{8}$$

In order to get $A(s)$ back to the time domain, we apply the inverse Laplace transformation to Eq. (8), and obtain

$$a(t) \propto b(t) + \tau\frac{d}{dt}b(t). \tag{9}$$

Here, we used a well-known theorem that the inverse Laplace transformation of $sB(s)$ is a differentiation $\frac{db(t)}{dt}$. Eq. (9) indicates that the excitation voltage profile $a(t)$, to be programmed in the NMR spectrometer, should include, in addition to the target profile $b(t)$, its time derivative $\frac{db(t)}{dt}$ as a correcting term, and should be their linear combination. Eq. (9) also tells that the relative contribution of the correcting term, which is zero for the steady state, is determined by the decay time constant $\tau = 2Q/\omega_0$ of the tuned circuit, and becomes important as increasing the Q factor and decreasing the frequency. This is quite consistent with the fact that deviation of the rf-pulse shape from the excitation voltage profile is large for high-Q probes and for experiments at low frequencies. Importantly, this result implies that no Q-damping is necessary to realize the intended rf-pulse shape, when one actively compensates the rf-pulse transients according to Eq. (9).

In order to examine the effectiveness of the pulse design according to Eq. (9), we consider a Gaussian target rf-pulse shape $b(t)$ with a width t_d, which is expressed as

$$b(t) = \exp\left[-4\ln 2(t/t_d)^2\right]. \tag{10}$$

Using Eqs. (9) and (10), we obtain the excitation voltage profile $a(t)$ that would result in the target Gaussian rf-pulse shape $b(t)$ as

$$a(t) \propto \left[1 - 8\ln 2(\tau t/t_d^2)\right]\exp\left[-4\ln 2(t/t_d)^2\right], \tag{11}$$

where the optimal weighting factor τ is expected to be the probe recovery time constant $2Q/\omega_0$.

Experimental studies were carried out as follows. A pickup coil was placed beside a sample coil of a home-built NMR probe tuned at 102.5 MHz. In order not to disturb the probe circuit, the position of the pickup coil was carefully chosen, so that the coupling coefficient between the pickup coil and the sample coil was less than 10^{-3}. The Q-factor of the probe was obtained to be 38.7 from least-square fitting of the frequency dependence of the measured S_{11} parameters by a Lorenzian function. Thus, the decay time constant τ was estimated to be $2 \cdot 38.7 \ (2\pi \cdot 1.025 \times 10^8 \text{ Hz})^{-1} \sim 120$ ns. The rf-voltage signal was created using an arbitrary waveform generator (AWG7102, Tektronics) and sent to the probe, and the resultant rf-field was detected by the pickup coil and monitored on a digital oscilloscope.

First, we examined the rf-pulse shape without active compensation by programming the excitation voltage profile to be a Gaussian function with a full width at half height of 118 ns. This excitation waveform is shown in Fig. 2a. As expected, the resultant rf-pulse shape monitored with the pickup coil was distorted with the transient, as shown in Fig. 2e.

We then monitored the rf-pulse shapes with the actively compensated excitation profile programmed according to Eq. (9) for various weighting factors τ. For the values of τ shorter than 120 ns, the transient tail of the pulse was reduced as increasing τ (Fig. 2b and f), and the rf-pulse shape satisfactorily coincided with the target Gaussian pulse when the weighting factor was set close to the decay time constant (120 ns) of the probe (Fig. 2c and g). When the weighting factor was further increased, the inverse transient tail appeared, which indicates the overcompensation (Fig. 2d and h).

The problem of probe ringing is more serious as decreasing the frequency, and has been tackled in low-field NMR and NQR experiments where the resonance frequency is about 10 MHz or less. On the other hand, in more popular experiments using much higher frequency, the recovery time constant of the probe is typically on the order of a hundred nanoseconds, which may appear to be short enough to cause no substantial disturbance without compensating the rf-pulse transients. Nevertheless, the importance of active compensation proposed in this work would revisit, considering the recent progress in NMR probes. For example, in cryo-coil probe, which is now widely available as commercial products for liquid-state NMR [10–14] and also recently reported for solid-state magic-angle spinning NMR [15], the Q-factor is significantly enhanced over that in the conventional probes.

Also, the approach presented in this work would find interest in experiments using a microcoil, where very strong rf-irradiation up to several MHz can be applied [16–19]. In order to fully exploit strong pulses realized in the microcoils, rf pulses have to be switched in a short period of time, and the effect of the pulse transients would be relatively serious even if the Q factor is in general not very high. In order to apply the idea presented here to such a case, an NMR spectrometer, together with an rf-amplifier, are re-

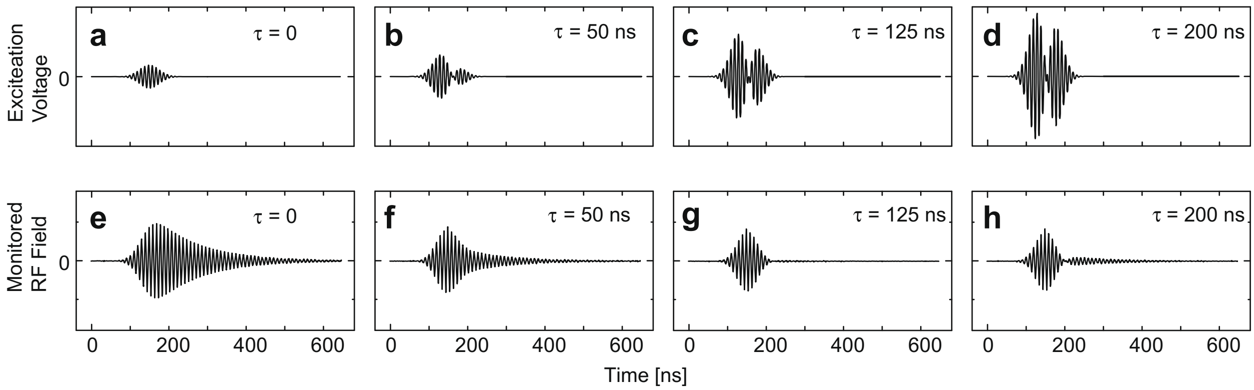

Fig. 2. Excitation-voltage waveforms for a Gaussian rf-pulse (width: 118 ns, carrier frequency: 102.5 MHz) (a) without active compensation, (b–d) with active compensation according to Eq. (11) for $\tau = 50$, 125, and 200 ns. The resultant rf-pulse shape monitored by the pickup coil are plotted in (e–h), respectively.

quired to be capable of controlling the rf-amplitude in a short time scale compared to that in current typical NMR experiments. In this sense, the present work suggests one possible direction toward which NMR hardware developers, both in academia and in industry, should direct. Modification of our home-built NMR spectrometer [20,21] for this purpose is now in progress.

To summarize, we have proposed a new concept of designing an excitation voltage profile back from an intended target rf-pulse shape. When the impulse response of the resonant circuit is approximated by an exponential function with a decay time constant given by its recovery time, the voltage profile of the excitation pulse, to be programmed in the NMR spectrometer, is formulated as a linear combination of the target rf-pulse shape and its differentiation, and the contribution of the latter is proportional to the time constant of the tank circuit. The validity of this formula has also been experimentally confirmed. Since the idea proposed in this work allows one to realize an arbitrary pulse shape without *Q*-damping, one can not only suppress the transient rf-pulse tail but also accurately design and implement rf pulses with sophisticated amplitude modulation. Apart from the amplitide transients, phase transients of rf pulses [22] are also of considerable concern, in particular for multiple-pulse sequences [23]. Active compensation of the phase transients based on the same idea proposed in this work is also underway.

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