Calculation of optimal parameters for $^{19}$F MRI

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Abstract. This paper presents a method for optimizing the parameters of the scanning pulse sequences for MRI in relation to objects with a wide NMR spectrum. In this case, a broadband excitation of the spin system is difficult because of hardware limitations. It is proposed to apply the selective excitation, the optimum parameters of which are calculated by an algorithm that uses information concerning the NMR spectrum. The method is especially useful for $^{19}$F MRI of fluorocarbons.

1. Introduction. Purpose

There is a problem of obtaining MR images of object with a wide NMR spectrum. This is especially true for the $^{19}$F MRI [1,2]. The wider is the spectrum the higher are requirements for transmitter power, gradient system strength, data sampling rate and receiver sensitivity. These requirements grow with increasing magnetic field. To solve this problem one needs to use narrow-band (frequency selective) excitation of the spin system. In this case it is necessary to optimize the scanning parameters - choose the excitation frequency and spectrum width. We made software that solves this task. It uses information about a specific NMR spectrum and calculates the scanning parameters which give the maximum MR signal. We used calculation results to optimize pulse sequences parameters in our $in vivo$ MRI studies which were carried out at 0.5- and 7-T scanners [3,4].

2. Materials and methods

The idea of the method is to calculate the signal of nuclear induction $S(t)$ for different variants of frequency selective excitation of the spin system - excitation frequency $f_0$, spectral width of excitation pulse $\Delta$ - and to select the optimal one. Search for optimal parameters ($t$, $f_0$, $\Delta$) is made within the intervals defined by technical limitations. It is assumed that they are known for the equipment on which it is planned to carry out MRI. Sorting out of variants is realized by specialized software that makes calculations in batch mode and gives the excitation parameters in which the maximum MR signal is realized.

Scheme of the method is shown on Figure 1. High resolution NMR spectrum $F(f)$ is multiplied by a Gaussian function $G(f)=G(f,f_0,\Delta)=\exp(-2\times(f-f_0)^2/\Delta^2)$. The result undergoes to inverse Fourier transform (IFT) that gives value $S(t)=S(t,f_0,\Delta)$. Then its magnitude $|S(t)|$ is calculated.

It is assumed that $|S(t)|$ determines the brightness of the pixels on the MR image. Therefore, the values of “$t$” which give extremes of the $|S(t)|$ serve as a reference points for setting the optimal TE
value of gradient echo pulse sequence (GE). The value of $|S(t)|$ at $t = 0$ determines the MR signal for spin echo pulse sequence (SE).

![Diagram](image)

**Figure 1.** The scheme of calculating the MR signal by the selective excitation.

The program creates a 3D array of $|S| = S(t, f_0, \Delta)$, and then searches for the two sets of parameters $(t, f_0, \Delta)$. One of them gives the maximum value for $|S|$, the second - for $|S| \cdot \Delta^{-1/2}$. The latter value is proportional to the signal-to-noise ratio ($|S|/N$) as the root mean square amplitude of the thermal noise N is proportional to $\Delta^{1/2}$. The range of variable parameters of frequency selective excitation is defined considering hardware limitations. The gradient system strength determines the minimum values of TE, the transmitter power and the permissible radiofrequency load determine maximum value of $\Delta$, as it is inversely proportional to the pulse length.

The method is most suitable for pulse sequences, which use Gaussian pulse (its length $\tau$ cut-off of 10% is calculated by the formula: $\tau = 2.74/\Delta$) with small flip angle (FA) [5]. These requirements can be easily fulfilled in the GE method. But the results of calculations can be demanded for the SE technique where the flip angles are 90° and 180°. However, in this case, the results of calculation should be used only for a rough estimate of the optimum parameters. In general, for accurate calculations instead of the Gaussian function $G(f)$ excitation profile calculated from the Bloch equations should be used, [3]. In addition, it is necessary to take into account differences in the longitudinal relaxation times for different spectral lines. Besides, to clarify the optimal TE for the SE method effects of transverse relaxation and J-modulation should be taken into consideration, therefore the experimental dependence of $|S|$ on TE should be measured.

### 3. Results

The method has been tested for fluorocarbon drug Perftoranum® [6]. Figure 2 shows its $^{19}$F NMR spectra which were obtained in the fields of 0.5 and 7 Tesla using the Bruker’s scanners – Tomikon S50 and BioSpec 70/30 USR. In addition to spectrum data we introduced into our program the limit values for $\Delta$ and TE, to reduce the range of variable parameters.

![Spectra](image)

**Figure 2.** Spectra of Perftoranum® at fields 0.5 and 7 T and the optimal parameters for the selective excitation of the spin system, defined according to the calculating algorithm.

Figure 2 shows the results of calculation - parameters TE, $f_0$ and $\Delta$, giving the maximum value of $|S|/N$ for the GE and the SE techniques. Vertical red lines indicate the points of the excitation frequencies with respect to the NMR spectrum. The lengths of the horizontal lines correspond to the optimum values of $\Delta$. As for the GE method, the value of $\Delta$ should be as small as possible. This value
is determined by technical limitations. For the method of SE optimum values \( \Delta \) correspond roughly to the width of the spectrum part in which the most intense lines are concentrated.

Calculated optimal parameters are of practical interest if a small deviation of them from the optimum values does not lead to a significant decrease of the MR signal. To estimate the stability of the optimal mode of selective excitation, we analyzed the behavior of functions \(|S|\) and \(|S|/N\) in the vicinity of their maximum values when two of the three parameters are fixed. Figure 3 shows the corresponding calculated (blue) and experimental (red) graphs for the GE and the SE modes.

![Graphs showing calculated and experimental values for GE and SE modes.](image)

**Figure 3.** Calculated (blue) and experimental (red) curves of \(|S|\) and \(|S|/N\) for GE and SE modes. Measurements were carried out on 0.5- and 7-T MRI scanners.

For the SE mode, the calculated values of \( S(t) \) are meaningful only for \( t \sim 0 \). Therefore experimental graphs \( |S(TE)| \) for the SE mode are shown to reveal \( J \)-modulation and \( T_2 \) decay. These factors should also be taken into account when calculating the optimum values of TE. Common values are: \( TR = 0.5 \) s, and \( FA = 30^\circ \) for the GE mode. Attention was drawn to the inadmissibility of the chemical shift artifacts on the MR image. Therefore, for the study \( |S| = |S(\Delta)|/N \) we installed sampling rate - receiver bandwidth (BW) - equal to \( \Delta \times N_r \), where \( N_r \) is number of frequency encoding steps. Typically, \( N_r \) was 64. In all other experiments we installed BW at maximal possible value - up to 0.2 and 1 MHz for 0.5 and 7 T scanners, accordingly.

It can be seen that the experimental graphs, in general, coincide closely with the calculated values. The largest discrepancy is noted only for the graph \( S(f_0) \) for the SE mode. This is due to the fact that \( TR = 0.5 \) s was comparable with the longitudinal relaxation times \( T_1 \), and these times are significantly various for the peaks belonging to the different components of the fluorocarbon compound. For the
method GE this factor is not significant, because FA is small. It may be noted that curves \(|S(Δ)|\) increase monotonically with increasing Δ. But for dependence of the signal-to-noise ratio \((S(Δ)/N)\) the situation is reversed. This is due to the fact that the NMR spectrum is not a band but is a set of narrow lines. Therefore with the increase of Δ, the total induction signal is growing slower than the thermal noise whose spectrum is continuous and its amplitude increases \(\sim Δ^{1/2}\). This does not exclude the presence of local extrema near Δ, comparable to the spectral width of the zone in which the most intense peaks are concentrated.

We used the results of the calculations when setting the parameters of MRI scanning in vivo studies using laboratory animals (7 T) and a human body (0.5 T) – figure 4. The combination of \(^1\)H and \(^{19}\)F images help to clarify the localization of fluorine relatively to anatomical structures. Sometimes the presence of fluorine can be detected on the \(^1\)H MR image by loss of signal (the rightmost fragment).

![Figure 4](image)

**Figure 4.** Left three fragments: \(^{19}\)F MRI (SE) shows accumulation of the drug Perftoranum® in the liver, spleen and thymus after intraperitoneal injection of the drug into the body of a rat. Right three fragments show the moving capsule filled by perfluorodecalin (main component of Perftoranum®) in the human gastrointestinal tract. \(^{19}\)F MRI (GE) is the sum of the images obtained at intervals of 0.5 to 1 hour. The total time of the study - 8 hours.

4. Discussion. Conclusion

The proposed method allows in relatively simple manner to calculate the optimal parameters of MRI scanning of objects with complex NMR spectrum considering hardware resources. The method can be adapted for more accurate calculations by using excitation profile calculated from the Bloch equations instead of the Gaussian function. Method efficiency is improved by adding information about the parameters of relaxation and spin-spin coupling constants.

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Page 3, Figure 3:

The published version of figure 3 is corrupted. This corrigendum contains corrected version of the image.

![Figure 3](image)

*Figure 3.* Calculated (blue) and experimental (red) curves of $|S|$ and $|S|/N$ for GE and SE modes. Measurements were carried out on 0.5 and 7 T MRI scanners.