Possibilities of using spectral analysis in method of nuclear magnetic spectroscopy for condensed media investigation

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Abstract. The necessity of developing a mathematical model for converting the recorded NMR signal using a modulation technique into the spectrum for conducting the composition of the medium under study is substantiated. A mathematical model has been developed to represent the NMR signal in the form of a spectrum, taking into account the features of its registration from condensed matter. Spectra of calculated and experimental NMR signals are presented. Their comparison is completed.

1. Introduction

The development of scientific and technological progress has led to the emergence of a large number of tasks, which need to be solved during the ecological monitoring [1-11]. The ecological monitoring need to be divided into several parts, because each part has its own data [11-16]. The greatest load is the analysis of various condensed matter, for example, in agriculture. Moreover, complex tasks are posed in these cases. For example, there is a study of the effect of a fungal infection on light reactions of soft wheat photosynthesis while simultaneously recording induction curves of fast and slow fluorescence, as well as the redox-state of the pigment P700 [17]. High resolution devices are needed to be solved them [3-6, 10, 18-21]. These devices do not need to be loaded with the work of monitoring condensed matter without deviations from the standard state, for this they use various methods of express control [3, 4, 16, 18, 19, 22, 23].

Currently, there is large number of different methods for conducting express control [3, 5, 18, 19, 23-29]. Most of them are designed to control a certain type of medium, such as water or gasoline [30, 31]. Recently, another additional requirement has been introduced to devices for express control. Measurements that are used for express control should not make changes in the physical structure and chemical composition of the test medium [2, 13, 19, 28, 32, 33]. The fulfillment of this condition is possible only in case of use for express control of devices with the work principle is based on the phenomenon of nuclear magnetic resonance (NMR).

The conducted research showed that during express control of the condensed medium state by NMR, the signal from its recorded with the using a modulation technique in a weak magnetic field. Other methods of the NMR signal detecting in a weak magnetic field in a small-sized magnetic system of the device do not allow reproducing the necessary measurement error.

2. Method for constructing the spectrum of NMR signals

The lack of the adequate theoretical model is one of the drawbacks of the modulation technique used for express control of the condensed medium. It does not allow reproducing of the line shape of the recorded
NMR signal in a weak field and determining the contribution between the absorption and dispersion signals in it. It need to be for determining the composition of the medium. In some cases, the measured values of the relaxation constants $T_1$ and $T_2$ are not enough to make a reliable decision. One of the possible solutions to the problem of determining the contributions to the recorded NMR from the absorption and dispersion signals is the use of spectral analysis. Therefore, the aim of this work is the developing a methodology that can reproduce the NMR signals spectra being recorded in conditions of weak magnetic field modulation in the interpolar space of a small-sized NMR relaxometer.

The results showed that the shape of the line $G(t)$ of the recorded NMR signal can be described by the following relation device [30-37], taking into account the features of the autodyne detector, as an integral:

$$ G(t) = F \left( \frac{A}{A+B} u^2(t) + \frac{B}{A+B} u^2(t) \right)^{1/2}, $$

where $u(t)$, $u(t)$ are the absorption and dispersion signals, $A$ and $B$ are the coefficients that determine the contribution to the recorded NMR signal from the absorption and dispersion signals, and $F(t)$ is the coefficient taking into account phase changes.

The absorption and dispersion signals for (1) are obtained from the solution of the Bloch equations written in a rotating coordinate system, taking into account the use of the modulation technique for recording the NMR signal [30-37]. The solution of these Bloch equations can only be obtained numerically. Then, the coefficients $A$, $B$, and $F$ are selected empirically. The latter depends on the temperature and composition of the medium. It makes express control time-consuming. It becomes less efficient and operational. Therefore, we propose to solve this problem using a spectral analysis of the absorption signals $u(t)$ and dispersion $u(t)$, they are obtained from solutions of the Bloch equations for (1). If we compare the spectra from the calculated signals $u(t)$ and $u(t)$ and the spectra from the experimental signal, we can determine the contributions of the absorption and dispersion signals to the recorded NMR signal.

The experimental signal and the calculated absorption and dispersion signals for water are shown in figures 1 and 2.

![Figure 1](image.png)

**Figure 1.** The NMR signals from water using a modulation technique.
The analysis of the experimental and calculated NMR signals (figures 1 and 2) showed that they cannot be described using periodic functions. Therefore, we propose using the discrete Fourier transform to construct the spectra of NMR signals, because these signals cannot be described by any periodic function:

$$y_k = \sum_{n=0}^{N-1} x_n e^{-j2\pi kn/N}$$

(2)

where \(n = 0, 1, 2, ..., N - 1\), \(x_n\) is the input data sequence, \(N\) is the number of elements of the input data sequence \(x_n\).

$$y_k = \begin{cases} y_0 & k = 0 \\ \sqrt{2} \frac{y_k}{N} & k = 1, 2, ..., \left\lfloor \frac{N}{2} - 1 \right\rfloor \end{cases}$$

(3)

In relation (3), the operation in brackets \([N/2 - 1]\) means rounding to the nearest smallest integer. Accordingly, the amplitude spectrum \(S\) is the modulus of the one-sided complex spectrum, the phase spectrum \(P(f) = \arg y_k\) is its argument, where \(f = k \Delta f\).

3. The results of the study of the structure of the NMR signal

The spectra (amplitude and phase) of an NMR signal recorded from a water sample obtained using relations (2) - (3) are presented on figure 3.
The spectra from the calculated waveform of the NMR signal of water (figure 2) is presented on figures 4 and 5.

Figure 4 (a, b). The spectra from the calculated NMR absorption signal for water: (a) amplitude; (b) phase.

Figure 5 (a, b). Spectra from the calculated NMR dispersion signal for water: (a) amplitude; (b) phase.

The analysis presented in figures 3-5 spectra shows that in the frequency range from -5 to 5 kHz they have the same dependence, both in amplitude and in phase.

4. Conclusion
The results obtained show that our new method of using spectral analysis allows us to obtain information on the contributions of the absorption signals and dispersion recorded by the NMR signal using a modulation technique from a condensed medium located in both stationary and current state. It allows one to study the structure of the line of the registered NMR signal from various parameters of condensed matter, as well as from the conditions for recording the NMR signal in various instrument designs, for example, in a small-sized NMR spectrometer during express control or NMR flowmeter-relaxometer.

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