On necessity for analytical solution of the Bloch equations for nuclear magnetic resonance signals at condition express control of liquid medium

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Abstract. The necessity of using express analysis methods to control medium condition is substantiated. It has been shown that the method of express control based on the phenomenon of nuclear magnetic resonance is one of the most preferable. It was found that to increase the information about the medium condition state obtained from the recorded NMR signal, it is necessary to use a mathematical model (based on analytical solutions of the Bloch equations). Two approaches are considered that are used to describe the NMR signal in a liquid medium. It is determined that in the classical approach in the system of Bloch equations it is possible to take into account the peculiarities of using radiotechnical methods of signal registration. The direction of the analytical solution of the Bloch equation is proposed. The experimental data are compared with the numerical solution.

1. Introduction

With the development of scientific and technological progress, the deterioration of the ecological state of the environment and other reasons, express control has become an important element in human life [1-9]. Nuclear magnetic resonance (NMR) is one of the promising methods of express control of liquid media at the sampling site [9-17]. Devices, the principle of operation of which is based on the phenomenon of NMR, do not make irreversible changes in the composition and structure of the studied medium [7, 8, 10-14, 18-26]. Liquid media after express control using NMR instruments can be examined using other instruments (to obtain confirmation of the identified deviations in the state of the medium). New requirements for express control methods create a number of problems. One of them is the low functionality of the NMR method under express control. From the measured values of the times of longitudinal \( T_1 \) and transverse \( T_2 \) relaxation of a liquid medium, it is possible to establish only the presence of deviations from the standard state in it [20, 22, 26-30]. The rest of the information about the medium, which is contained in the recorded NMR signal using the modulation technique, is extremely difficult to obtain.

One of the main reasons that does not allow this is the lack of an adequate model for describing the recorded NMR signal using a modulation technique. Its development requires an accurate analytical solution of the Bloch equations with respect to absorption and dispersion signals, with coefficients that
take into account the registration of an NMR signal in a weak magnetic field using a modulation technique.

Only in this case it is possible to take into account the phase change with time in the recorded NMR signal by an autodyne detector.

2. System of Bloch equations for the case of recording an NMR signal using a modulation technique

The system of Bloch equations in a rotating coordinate system is represented in the following form [31-34]:

\[
\begin{align*}
\dot{u} + \frac{u}{T_2} + v \Delta \omega &= 0 \\
\dot{v} + \frac{v}{T_2} - u \Delta \omega &= -|\gamma|H_1 M_z \\
M_z + \frac{M_z}{T_1} - |\gamma|v H_1 &= \frac{M}{T_1}
\end{align*}
\]

(1)

This integral equation (3) is solved by the method of successive approximations [31]. The constructed solution can be interpolated. Interpolation of the response waveform by various orthogonal systems of functions and analysis of interpolation errors will be performed. Other approximal solutions of Bloch equations do exist [31, 35, 36].

Before substituting new coefficients (4) and (5) into equation (1), it is necessary to take into account one more feature of recording an NMR signal in a weak field. The NMR signal should be recorded only at the resonance frequency \(\omega_{\text{nmr}} = \omega_0 = \gamma H_0\). This is due to the small volume of the investigated medium, from which the NMR signal is recorded. If the frequency of recording the NMR signal \(\omega_{\text{nmr}}\) is detuned from the resonance frequency \(\omega_0\), the signal-to-noise ratio (S/N) can become less than 1.3. Accumulation of the NMR signal at this S/N ratio is impossible. Without accumulation, it is extremely difficult to learn the S/N > 3 ratio and carry out measurements with an error of no more than 1%. When this feature is fulfilled, formula (4) is transformed into the following function:
\[ \Delta \omega = \gamma H_m \sin(\omega_m t) \]  

(6)

After substituting (5) and (6) into (1), the Bloch equations are transformed into:

\[ \begin{cases} 
\frac{du(t)}{dt} + \frac{u(t)}{T_2} + \gamma H_m \sin(\omega_m t) u(t) = 0 \\
\frac{dv(t)}{dt} + \frac{v(t)}{T_2} - \gamma H_m \sin(\omega_m t) u(t) + \gamma H_1 M_z(t) = 0 \\
\frac{dM_z(t)}{dt} + \frac{M_z(t)}{T_1} - \frac{H_0 + H_m \sin(\omega_m t)}{T_1} - \gamma H_1 u(t) = 0 
\end{cases} \]  

(7)

In Bloch equations (7), there appear coefficients with a time term \( \gamma H_m \sin(\omega_m t) \). In this case, it becomes difficult to implement the classical solutions of equations (7). Namely, transform (7) by the method of Gvozdover and Magazanik [31, 35] into the integral form of Voltaire. Expansion in a series with the identification of the convergence condition (\( \gamma H_m^2 T_1 T_2 < 1 \)) is also not acceptable. It should be noted that the condition for the convergence of the series is the implementation in an NMR meter (small-sized) of fast adiabatic passage through resonance. It is extremely difficult to provide it in it when registering an NMR signal in a weak (magnetic) field.

Therefore, a number of the author began to implement new approximations and assumptions, for example \( H_0 \gg \gamma H_m \sin(\omega_m t) \). This assumption assumes that, when considering (2.6), the effect of modulation on the (constant) field \( H_0 \) is very small - in principle, it can be neglected. This approach made it possible to solve equations (7). This solution is very similar to the solutions obtained in [31–35]. Further, a term is added to the solution itself. With this term, a number of authors decided to take into account the modulation. If we analyze all such solutions, then we can choose the most adequate of them to describe the configuration of the NMR signal. In [36], this is presented:

\[ U = U_0 \exp\left(-\frac{1}{T_2} t\right) \cos(\omega_0 t + \frac{1}{2} \gamma \frac{dH}{dt} t^2) \]  

(8)

In a weak field, for adequacy, it is necessary to transform (8), taking into account (4), into a new relation:

\[ U = U_0 \exp\left(-\frac{t}{T_2^*}\right) \cos(\omega_0 t + \frac{1}{2} \gamma H_m \omega_m \cos(\omega_m t) t^2) \]  

(9)

The resulting relationship was also used to describe the recorded NMR signal in a weak field.

3. Description of NMR signal lines and their comparison with experiment

For example, figure 1 shows the experimental NMR signal from water (temperature \( T = 14.4 ^\circ C \)) and the result of its simulation using (9)

![Figure 1. NMR waveform from tap water. Line 1 corresponds to experiment. Line 2 – theoretical analysis](image-url)
The results obtained show a large difference between the experimental signal and the theoretical calculation. At the bottom of the dependencies, there is a complete mismatch. This is mainly due to the absence of the magnetic field parameter $H_1$ in ratio (9). This field is generated in the autodyne registration coil. It plays a primary role in determining the conditions for passage through resonance. Without taking it into account, it is impossible to obtain an adequate value of the parameters for the maximum of the $S/N$ ratio at the output of the registration circuit in a weak field.

To determine the adequacy of our proposed Bloch equations (7) for describing the NMR signal in a weak field, a mathematical model was developed for the numerical solution of equations (7). Equations (7) were solved for the components $u(t)$, $u(t)$, and $M_z$ under the following initial conditions: $u/|t=0| = u/|t=0| = 0, M_z/|t=0| = M_0$. The values of the relaxation constants $T_1$ and $T_2$ were determined from the recorded NMR signal. These $T_1$ and $T_2$ values were used to calculate the absorption and dispersion signals. Figure 2 shows the recorded NMR signal from tap water at a temperature $T = 293.3$ K.

![Figure 2. NMR waveform from tap water.](image)

Figure 3 and figure 4 show the calculations of absorption and dispersion signals for tap water.

Analysis of the obtained dependences figure 3 and figure 4 show that they reflect the nature of the physical processes corresponding to the experiment. However, additional calculations have shown that with an increase in $t$, every $T_m/2$ changes in the phase of the components $u(t)$ and $u(t)$ by $180^\circ$, as well as a sharp decrease in the values of the peak amplitudes. In real experiments, the same NMR signal is recorded by the autodyne every half-period $T_m/2$. Comparison with experiment can be carried out only within the first peak, since the phase is not taken into account.

Difficulties also arise in the interpretation of the resulting NMR signal (experimental), which consists of absorption and dispersion signals. It is necessary to enter a factor that takes into account the phase change. This coefficient has to be selected for each case, which is very difficult. The greatest agreement is achieved at the same contributions of the absorption and dispersion signals to the generated NMR signal. Figure 5 shows this signal.

In other cases of modeling, it is necessary to constantly select a coefficient that takes into account the phase of the signal and the coefficients of the contributions of the absorption and dispersion signals. It takes a long time. In the conditions of conducting research in express mode, such time costs are excluded.

This can be excluded only by obtaining an analytical solution to the Bloch equations. This problem is supposed to be solved using the Matlab software package used for technical computing tasks.

4. Conclusion
The preliminary results obtained showed that the direction we have chosen to expand the functionality of using express control using an NMR signal is promising. The analytical solution of the Bloch equations will take into account the phase of the NMR signal and delineate long-term studies of media using the modulation technique.
Figure 3. Calculated line shape of the absorption signal from water.

Figure 4. Calculated line shape of the dispersion signal from water.

Figure 5. The result of modeling the NMR signal line for water.

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