Peculiarities of magnetic resonance signals processing during the express control of the liquid media state

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Abstract. The paper discusses the need to develop a new approximation of the nuclear magnetic resonance signals. This approximation allows enhancing functional capabilities of express control devices. The universal mathematical model is developed to describe the shape of the NMR signals taking into account the peculiarities of their registration using a modulation technique in a weak field. The modeling results obtained are compared with experimental data.

1. Introduction
At present, one of the urgent tasks of applied physics is the development of fast and reliable methods of express control of the state of condensed media [1-7]. Now, the main requirement for express control methods is that research or measurements by these methods should not change the physical structure and chemical composition of the studied medium [4, 7-13].

The results of numerous experiments have shown that the method based on the phenomenon of nuclear magnetic resonance (NMR) is the only one that does not cause irreversible changes in the structure and chemical composition of various condensed matter, unlike optical, ultrasonic, X-ray, electromagnetic or other methods [2-4, 6, 7, 11-16]. In addition, this NMR method suitable for a large number of media, because the only condition for its use is the presence of nuclei with magnetic moments in the medium [4, 6, 17-22]. There are many of such media, especially among liquid ones, which contain protons in 99 % cases of their use.

Earlier we have developed compact NMR spectrometer and relaxometer based on the modulation technique [23-27]. Those devices were capable of investigating various media in the express mode. Unfortunately, during the express control, it is not always possible to register a full spectrum of the medium. In that case, you can make a decision using only the times of the longitudinal $T_1$ and transverse $T_2$ relaxation of a condensed medium. Having this information, it is possible to determine the deviation of the medium state from the standard one. However, the experience of express control of various media, especially hydrocarbon, showed that information about the deviations itself is not always enough to make a reliable decision on the further use of the medium. Often there are situations when it is necessary to establish what could have caused the deviations in the environment. One of the possible solutions to this problem may be the processing of the recorded NMR signal in the form of a damped non-periodic oscillation — “wiggles”. The form and structure of this signal differs significantly from the classical NMR signals recorded using high resolution pulsed NMR spectrometers and relaxometers placed in stationary specialized laboratories. The developed theories...
for describing NMR signals recorded in them based on the Bloch equations cannot be used for NMR signals recorded using a modulation technique in a weak field. This is because various approximations are made in these theories. Those approximations do not correspond to the conditions of NMR signal registration in a weak field. Currently there is no qualitative theoretical model for describing these signals.

Therefore, we propose to develop a mathematical model that allows describing the shape of the image (on the screen of a laptop or tablet during express control) of the NMR signal recorded in a weak field, taking into account previously established features [11, 19, 20, 24, 26, 27]. Then, using this model, it is possible to “decipher” the recorded signal and obtain the necessary information about the state of the environment and the causes of deviations in it.

2. Mathematical model of the recorded NMR signal

In the case of using a modulation technique for registering an NMR signal in a weak magnetic field, the value of $H$ changes as follows [19, 23, 26-28]:

$$H = H_0 + H_m \sin(\omega_m t)$$  \hspace{1cm} (1)

where $H_0$ is a constant magnetic field, $H_m$ is a modulation coil field, $\omega_m$ is a modulation frequency.

The closest equation that reflects the shape of the NMR line recorded in the experiment using the modulation technique was obtained in [29-32]:

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

Taking into account (1) equation (2) takes the following form:

$$U(t) = U_0 \exp\left(-\frac{t}{T_2}\right) \cos\left(\omega_0 t + \frac{1}{2} \gamma H_m \omega_m \cos(\omega_m t) t^2\right)$$  \hspace{1cm} (3)

Analysis of the obtained line shape using (3) shows that the recorded NMR signal does not depend on the value of the $H_1$ field, which is the determining parameter when it is registered by the autodyne detector. For recording the NMR signal with the maximum S/N ratio from different media, the value of $H_1$ will be different for different media, but there is no such dependence in (6). Figure 1 shows the registered NMR signal from water and the result of calculating its shape using (3).

![Figure 1](image_url)  

**Figure 1.** The NMR signal from water at a temperature $T = 291.4$ K. Graph 1 is the experimental data, graph 2 is the theoretical calculation of the line shape.
The calculation result presented in figure 1 (graph 2) using (6) has a significant discrepancy to the experiment (graph 1). Such discrepancies with the experiment confirm the incorrectness of its use (3).

Based on our previous experimental results, as well as data on studies conducted by other scientists in the field of NMR, expressions for envelopes can be represented in the following form:

\[
\begin{align*}
\bar{u}(t) &= \cos(g(t - f) + h(t - f)^2) \cdot \frac{1}{2} \left( \frac{a \exp(b t) - c \exp(-d t)}{a \exp(b t) + c \exp(-d t)} \right) \\
&+ \frac{1}{2} \left( \frac{a \exp( -b t) + c \exp(-d t)}{a \exp( -b t) + c \exp(-d t)} \right),
\end{align*}
\]  

(4)

where \(a, c\) are dimensionless parameters, \(b, d\) are attenuation coefficients \((b \sim 1/T_2, d\) takes into account the inhomogeneity of the magnetic field \(H_0)\), \(g\) is a parameter having frequency dimension \((Hz)\), takes into account the resonance frequency \(\omega_0\), \(h\) is a parameter having dimension \(1/s^2\), takes into account the modulation of the field, \(f\) is a parameter that has the dimension of time, necessary to correct the approximation in the time axis, because the first peak of the real signal is not always set to 0.

3. Results and their discussion

Figures 2 and 3 show, as an example, the result of comparing the shape of the peaks (“wiggles”) of the recorded NMR signal (graph 1) with the approximation of their shape (graph 2), made using for kerosene (figure 2) and gasoline AI-95 (figure 3). Exponential envelopes are also marked in both figures (graphs 3 and 4).

![Figure 2. The shape of the NMR signal from kerosene](image-url)
4. Conclusion

It was established that during the express control, approximation (4) can be successfully used. However, it should be noted, that this model has some restriction. It should be used if the qualitative composition of the mixture is known in advance and there is data on the preliminary graduations of all parameters included in (4), since they depend on the values of the magnetic fields $H_1$ and $H_m$, modulation frequency $\omega_m$, etc. Calibration should be performed for different nucleus of the medium, which will be used to record the NMR signal and temperatures. In the absence of this information it is impossible to use approximation (4).

The results obtained during the express control of various media, showed the reliability of the developed mathematical model and the validity of its application.

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