Detection of Nitrogen Substances by Nuclear Quadrupole Resonance in Large Volumes

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Abstract— In this work, we describe the design of a sensing system for the NQR detection of nitrogen substances in a large inspection volume. The system consists of a *Tecmag Scout* NQR console, *Tomco* linear amplifier (4 kW), a large distance/volume RF probe (either planar gradiometer or toroidal coil), a duplexer and a high-power Q-factor spoiler. We studied the conditions for optimal unilateral detection at distances up to 20 cm as well as for the detection inside a large volume. It has been shown that depending on RF probe configuration and ambient RF noise level), a ^{14}N NQR signal of a small amount (100 g) of hexamethylenetetramine (HMT) as the reference nitrogen substance can be detected using both types of RF detectors. Furthermore, a possibility of NQR detection for a partially shielded HMT sample has been also shown. The influence of conducting bodies near an NQR sample for detection performance has been studied as well. We have also demonstrated that this system can be applied to the detection of ammonium nitrate.

1. INTRODUCTION

Nuclear quadrupole resonance (NQR) is one of the prospective methods for the remote detection of nitrogen-based explosives and narcotic substances [1–4]. The advantage of this method is that the nuclear quadrupole resonance spectrum is unique for each chemical compound. The detection of even one line of the spectrum is sufficient for the identification of a substance. However, NQR is characterized by a relatively low signal-to-noise ratio and a high influence of outside radiofrequency interference. Identification of substances for the needs of transport security and industry is realized in conditions which are far from the laboratory ones. A substance to be detected may occupy only a small part of the scanned volume, it may be partially shielded, and a scanned volume may contain conductive parts, etc. Therefore, the development of efficient approaches for distant or large-volume NQR detection is a non-trivial issue. Signal-to-noise ratio (SNR) in NQR and nuclear magnetic resonance is defined by several factors, such as quality factor Q, the resonance frequency, filling coefficient $\xi = v_s/V$ (v_s is sample volume, V is a probed [RF probe] volume) and some others [5]. The main disadvantage of a large-volume coil is a very small value of $\xi (\ll 1)$. In experiments, this disadvantage is compensated by using coherent accumulations of signals, processing, and increasing the quality factor Q (because the SNR is proportional to $\sqrt{Q}$).

In this report, possible approaches for the detection of nitrogen-based substances in large volumes by the NQR method have been proposed. The conditions of work of the NQR detection system, which are close to real ones have been tested and their impact on the possibility of identification of nitrogen compounds has been estimated.

2. EXPERIMENTAL METHODS

The NQR system consists of a Tecmag Scout console (0.1–100 MHz), a Tomco BT04000-AlphaC power amplifier, a low-noise preamplifier Miteq (0–100 MHz), a home-made duplexer and a home-made Q-spoiler. Two possible designs of radiofrequency (RF) probes have been manufactured. The first one is a distant RF probe based on a planar gradiometer with sizes of about 50×30 cm made of 12 turns of copper wire with a diameter of 1 mm glued to a reinforced polyamide plate with a thickness of 5 mm (Fig. 1(a)). The gradiometer resonance frequency is near 500 kHz. The second one is a large-volume toroidal coil (shown in Fig. 1(b)). The one-turn toroid with sizes (of $170 \times 100 \times 50)\,\text{cm}^3$ is made of copper foil with a thickness of 0.1 mm. The volume used for the

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(a) (b)

Figure 1: The photo of (a) the gradiometer and (b) toroidal coil.

NQR detection in the gap of this coil is $50 \times 50 \times 55$ cm. The resonance frequency of the RF probe is tunable in the range of ± 5 kHz near the resonance frequency (3.31 MHz).

The loaded quality (Q) factor for the gradiometer coil was measured to be about 160, while that for the toroid coil was about 180. For the experiments, we used the sample of hexamethylenetetramine (HMTA, $C_6H_{12}N_4$) with a ^{14}N NQR frequency of 3.306 MHz at room temperature and ammonium nitrate (AN, NH_4NO_3, fertilizer granules produced by Gübretaş) with an NQR frequency of 0.497 MHz at room temperature [4].

3. FEM SIMULATIONS

Prior to manufacturing, the distribution of the magnetic field component of the radiofrequency (RF) field near the gradiometer coil and inside the coil gap for the toroid probe was modelled by the finite element method (FEM). Comsol Multiphysics software package has been used in the modelling. The calculated distribution of the RF field of the gradiometer coil is presented in Fig. 2. The distribution of the RF field of the toroidal probe is presented in Fig. 3.

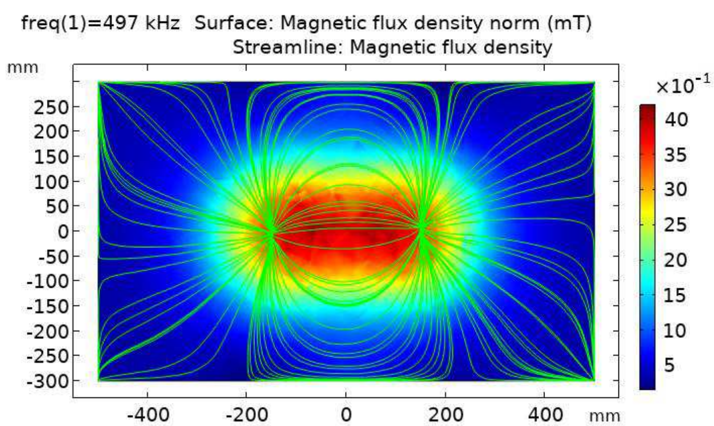


Figure 2: Magnetic field distribution near the unilateral gradiometer: the field induction in the section parallel to the plane of the gradiometer (the (x, y) plane) at a distance of 15 cm. The dark blue colour corresponds to the minimum field.

It is known that the optimal (90°) pulse duration in NQR is given by condition of $\gamma B_1 t_p = 0.66\pi$, where γ is the gyromagnetic ratio of ^{14}N nuclei, B_1 is the magnetic field induction, t_p is an NQR radiofrequency pulse duration [4]. Thus, using the typical values of the optimal pulse duration in the NQR experiments (e.g., $t_p = 200\,\mu s$ and $300\,\mu s$) we estimate the average value of the AC magnetic field induced near the RF probe to be about 3.3 mT and 2.2 mT, respectively.

The results of the simulations presented in Fig. 2 show that the optimal distance for the pulses with the power of 2 kW is limited by the distance of 15 cm. For larger distances, it is necessary to increase the pulse power and the quality factor.

It is obvious that much larger detection distances can be obtained for a toroidal RF probe, although, owing to a larger detector size.

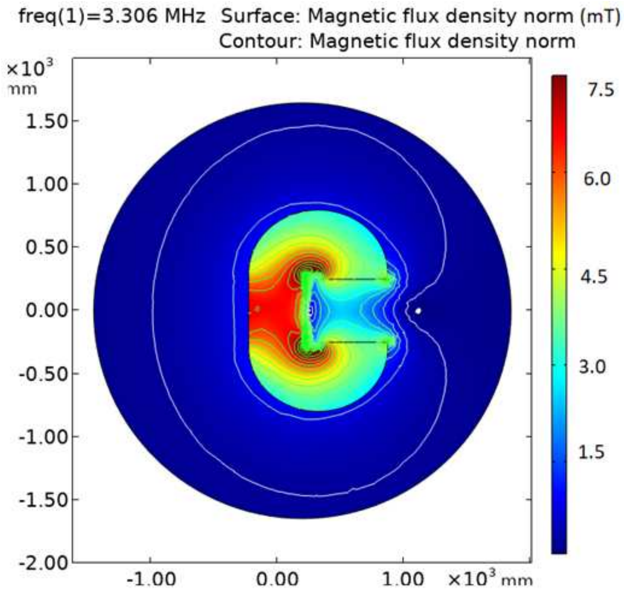


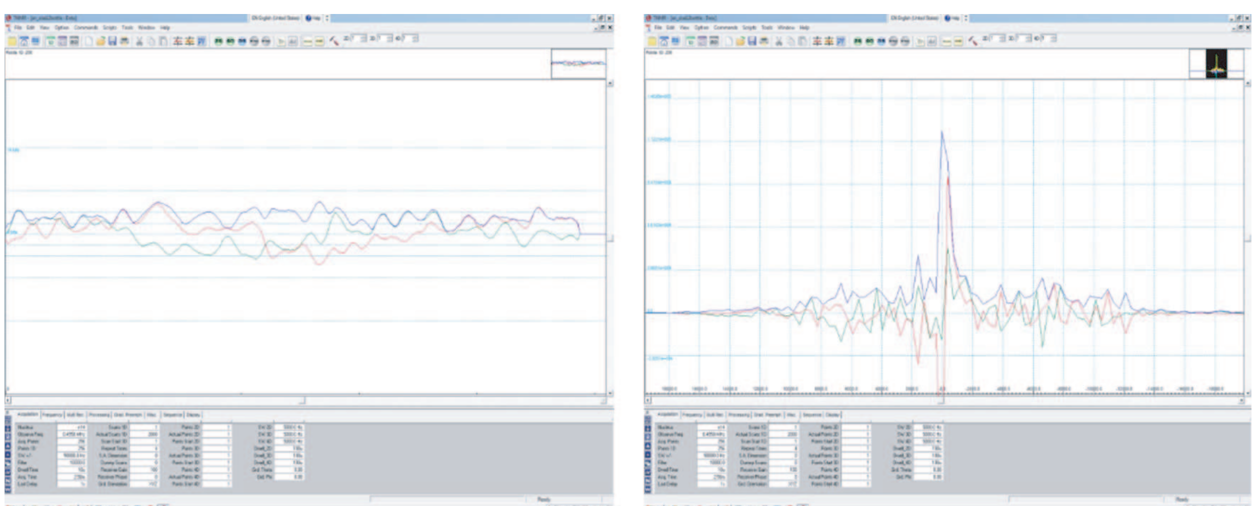
Figure 3: Magnetic field distribution in the one-turn toroid coil: the field induction in the longitudinal section (dark blue colour corresponds to the minimum field).

4. EXPERIMENTAL RESULTS

4.1. Planar Gradiometer

The weight of the sample for robust detection of the NQR signal strongly depends on the position in the lateral plane (parallel to the gradiometer probe plane) as well as on the distance from the gradiometer plane. The accumulation time was in the interval of 1–2 minutes. The NQR signal as a function of the distance from the gradiometer plane is presented in Fig. 5.

The measurement results of AN signals are presented in Fig. 4. A gradiometric coil consisting of two square coils was used as the probe (Fig. 1(a)). The loaded quality factor is greater than 160. The sample weight of the AN sample is between 1 kg and 2 kg.



(a) (b)

Figure 4: (a) Time domain NQR signal of AN and (b) Fast Fourier Transform of NQR signal.

4.2. Toroidal Probe

A minimal weight of the HMT substance for robust detection of the NQR signal was determined for the accumulation time (i.e., time of detection) in the interval of 1–2 minutes. We defined that the sample with a weight between 100–500 g of HMT can be detected depending on the position of

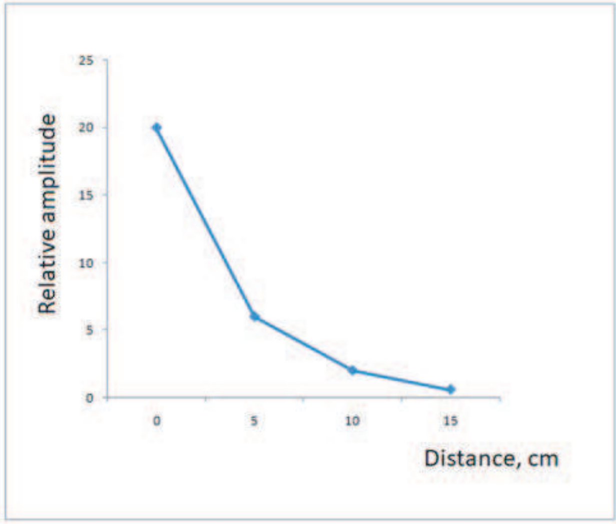


Figure 5: The NQR signal as a function of the distance from the gradiometer plane is shown.

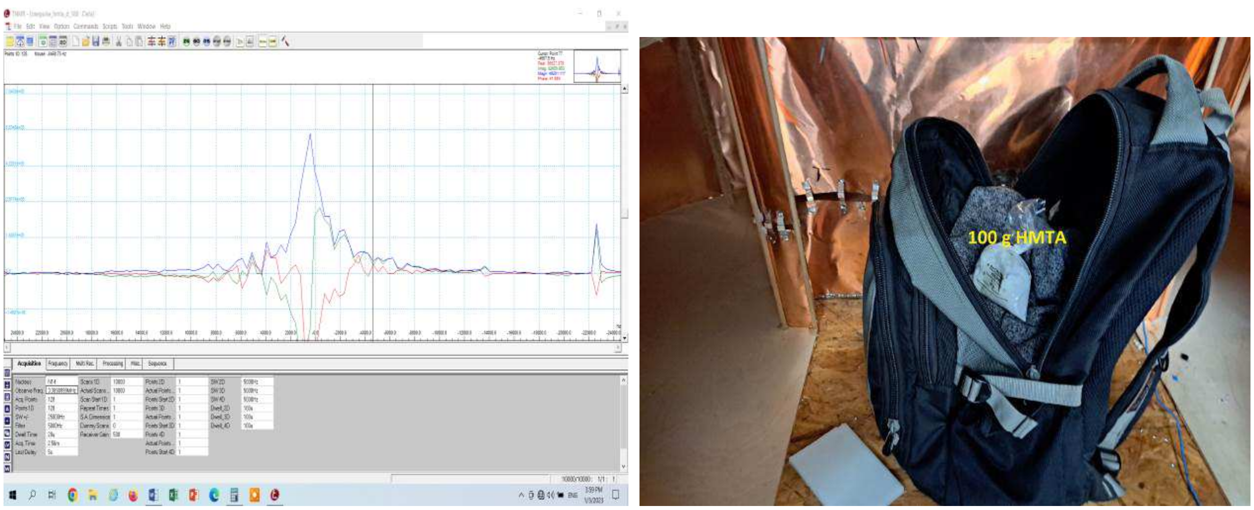


Figure 6: The NQR signal detected for the 100 g of HMT in the center of the toroid RF probe is shown.

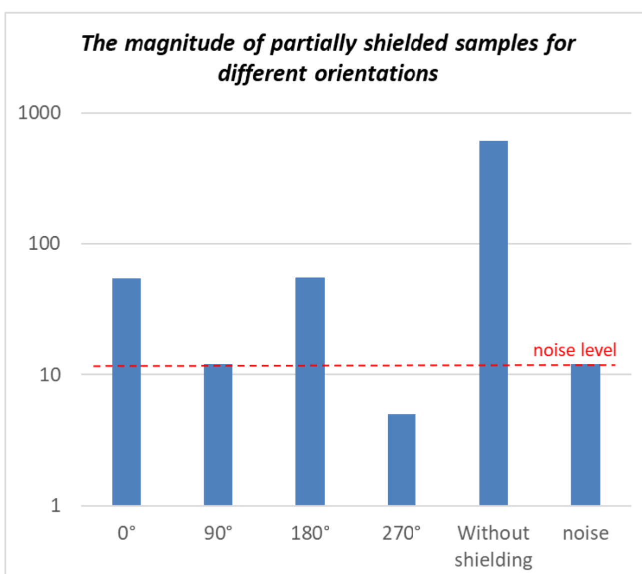


Figure 7: The signal intensities in the *logarithmic scale* as a function of the window orientation relative to the central axis of the toroid opening are shown as a circle diagram.

the sample. The typical NQR signal is presented in Fig. 6. The sample of smaller weight can be detected by increasing the detection duration or by increasing the quality factor of the RF probe. We have also tested the influence of shielding the sample with foil on the possibility to detect NQR signals. We have established that wrapping the sample with a weight of 2 kg with a single-turn aluminium foil is enough to shield the NQR signal from the HMT sample. However, the sample with a weight of 2 kg wrapped with a single-turn aluminium foil can be detected if a square hole with an area of $100\,\text{cm}^2$ persists in the sample shielding.

The signal intensities depending on the window orientation relative to the central axis of the toroid opening are presented in the logarithmic bar plot in Fig. 7. The time of each measurement given in Fig. 5 was nearly 8 minutes. It is clear that 0° and 180° orientations provide the maximum possible signal with respect to other geometries.

5. CONCLUSION

Two possible designs of a sensing system for the NQR detection of nitrogen substances in a large inspection volume have been manufactured and studied. A large-distance RF probe based on a planar gradiometer and a large-volume toroidal coil have been tested. For the planar gradiometer, we have studied the conditions for optimal unilateral detection of AN at distances up to 15 cm, while for the toroidal coil, we have studied the conditions for the detection of HMT inside a large volume (~ 107 litres) and the sample filling factor of the probe $\xi \approx 0.02$. It has been shown that a ^{14}N NQR signal of a small amount (in the range of 100–500 g depending on the RF probe configuration and ambient RF noise level) of HMT can be detected. Furthermore, a possibility of NQR detection for a partially shielded HMT sample has been also shown. The influence of conducting bodies near an NQR sample for detection performance has been studied as well.

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