Detection of NQR signals using wavelet transform and adaptive filters

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Abstract: NQR signal processing method based on two adaptive filters techniques namely adaptive noise cancellation (ANC), adaptive line enhancement (ALE) and wavelet transform are studied and it is shown that ALE is faster detection method with improved signal to noise ratio. Based on the ^{14}N NQR signal observed from $NaNO_2$, ALE seems to be easier and more reliable technique for NQR spectroscopy.

Keywords: nuclear quadrupole resonance; NQR; nuclear magnetic resonance; NMR; wavelets; adaptive line enhancement; ALE; adaptive noise cancellation; ANC.

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1 Introduction

Nuclear quadrupole resonance (NQR) is solid state radio frequency technique that can be used to detect the presence of quadrupolar nuclei that are present in many drugs, narcotics and explosives (Garrowway et al., 2001). NQR provides a unique signature of the material of interest. The NQR signal depends on the chemical structure of the molecule. Hence, in the case of land mine detection, NQR detects the ^{14}N of the explosive, without suffering interference from, any nitrogen-based fertiliser in the soil. The NQR frequencies for explosives are quite specific and are not shared by other nitrogenous materials. NQR is related to nuclear magnetic resonance (NMR) and Magnetic Resonance imaging, but does not require a large static magnetic field to split the energy level of nuclei. This makes it attractive as non-invasive technique to detect explosives in landmines and screening baggage for explosives at airport (Gudmuundson et al., 2009).

Conventional techniques such as EMI or GPR sensors for this type of detection have numerous false alarms (Garrowway et al., 2001). The pure NQR of ^{14}N nuclei is a promising method for detecting explosives in the quantities encountered in landmines.

An FPGA-based NQR spectrometer for detection of nuclei ^{14}N (frequency range up to 6 MHz) has been designed, constructed in ED, BARC (Hemnani et al., 2014) is shown in Figure 1. The stable nitrogen ^{14}N has natural abundance of 93.6% and nuclear spin $I = 1$ with its associated nuclear electrical quadruple moment. The ^{14}N NQR transitions in various solids fall in the frequency range 0 to 6 MHz (Rudakov and Belyakov, 1998), hence the choice of the frequency band of our spectrometer.

The main challenge for NQR techniques is the extremely poor signal to noise ratio (SNR). To improve SNR, many repetitions of the experiment are necessary. The most commonly method is to use repeated single RF pulse and acquire NQR signal after each pulse. The rate at which RF pulse has to be repeated depends on physical parameters of nuclear relaxation which are spin-spin relaxation and spin lattice relaxation. Spin lattice relaxation time is denoted by T_1 determines the time necessary to regain its original thermal equilibrium state and gives bound to how quickly a pulse sequence can be repeated. The spin-spin relaxation time denoted by T_2 indicates decoherence and thus determines the RF pulse length. In practice we can apply a pulse sequence of length T_2 and repeat the pulse sequence every T_1. For most of explosives the relaxation times are very long which lead to long detection times (Garrowway et al., 2001).

^{14}N NQR signal was observed from $NaNO_2$. Even after utilising FIR filter the signal which was obtained was fully merged with noise. The SNR was improved by accumulation of 1,024 times and the signal is shown in Figure 2, however this method requires acquisition of large amount of data and is a time consuming procedure.

As we cannot shorten the relaxation times, much effort has been put into increasing the sensitivity of receiver and improving signal detection technique. To improve SNR per unit time several other techniques have been used, i.e., FIR filter (Rudakov, 2009), wavelet transform (Deas et al., 2004), and adaptive filter (Barall et al., 2005).

FIR filter is generally based on prior knowledge of spin echo. Wavelet transform is not suitable due to computational complexity. Adaptive filter algorithms are used in this work as these do not need prior knowledge of signal and also parameters of adaptive filter changes to meet the optimisation parameters.

Figure 1 Schematic diagram of FPGA-based NQR spectrometer (see online version for colours)

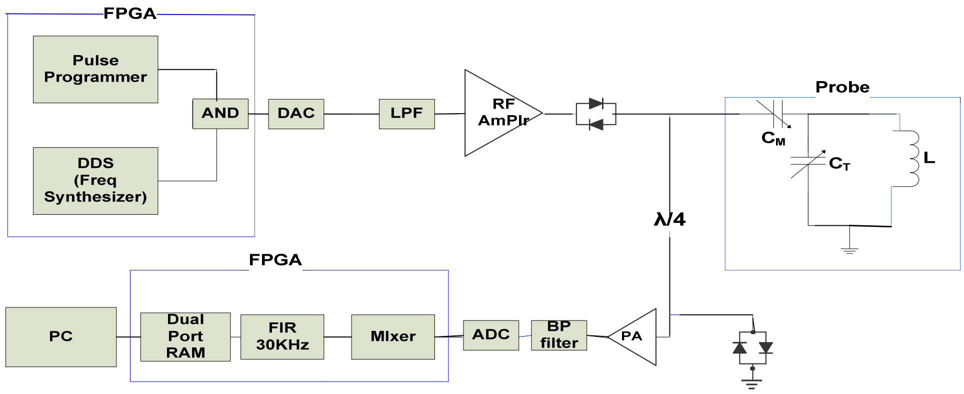
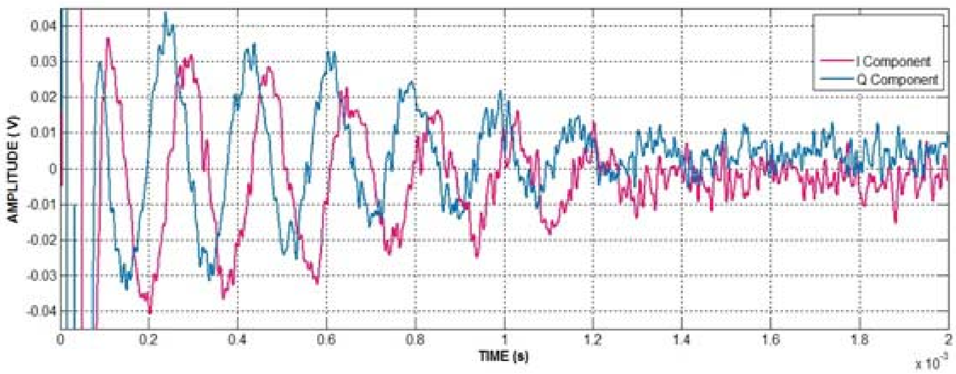


Figure 2 ^{14}N NQR signal (see online version for colours)



Note: *I* – in phase, *Q* – quadrature component

2 Wavelet denoising

Wavelet, filter bank and multi-resolution are used independently in field of signal processing (Vetterli, 1992). Wavelet decomposes the signal in to different frequency band and de-noising is done in each frequency band. The efficiency of wavelet transform over Fourier Transform is compared by Mozzhukhin and Molchanov (2005) and they proved that wavelet transform is better than Fourier transform for NQR response in terms of noise removing. They showed result of Donoho-Johnstone method for selecting threshold value for de-noising. De-noising is performed on every detailed coefficient.

Nagendra (2011) has shown that how non-stationary ECG signal is represented in time and frequency domain together by wavelet transform. Soft and hard thresholding can be used for wavelet transform de-noising (Hawwar et al., 2002; Donoho et al., 1993). Four different thresholding methods, like Minimax criterion, Sqtwolog criterion, Rigrsure and Heursure are compared and stated the best one by Neema (2012).

Traditionally, Fourier transform is used for frequency selective filtering to remove the noise but such filters may fail when noise shares the same frequency band with signal. Wavelet transform is powerful tool in such cases because it provides multi-resolution analysis of same signal.

In wavelet transform signal is decomposed into low frequency and high frequency components, where low frequency components are basically signal part, called as approximation coefficient and high frequency components are noise part, called detailed coefficient. Wavelet de-noising is done by soft and hard thresholding on wavelet transform coefficients. There are mainly three steps involved in wavelet thresholding.

- Decomposition: Signal is decomposed in approximation and detailed coefficients. The approximation coefficients are still further decomposed into next level of approximation and detailed coefficients. This process is repeated till desired level N is achieved.
- Detailing: For each level 1 to N, a threshold value is determined and thresholding is done on each detailed coefficients. It removes the noise content at each levels of detailed coefficient.
- Reconstruction: Filtered signal is reconstructed with modified detailed coefficients and approximant coefficient. Thus reconstructed signal is filtered at different frequency scales.

3 Adaptive filters

An adaptive filtering algorithm involves two basic operations filtering and updating. These two operations work interactively with each other. Both FIR and IIR filters can have adaptive property but due to stability issue FIR adaptive filter are used. An adaptive noise canceller (ANC) based on adaptive algorithm is used for noise reduction and weak signal extraction (Rudakov and Belyakov, 1998; Jakobsson et al., 2006; Tan et al., 2004; Smith et al., 2003; Garroway et al., 1997; Somasundaram et al., 2008). Adaptive line enhancement (ALE) is another form of ANC which needs only one input channel to detect the signal interfused by background noise which depends on principle of different autocorrelation between the signal and noise after time delay.

ANC and ALE are two adaptive filtering systems with similar mechanisms but slightly different designs (Ramli, 2012). ANC has two sensors to receive target signal and noise separately. The primary signal d(n) consists of signal and noise N_o together and reference signal x(n) is noise N_I, which is uncorrelated to signal but correlated to noise No. The reference signal passes through the adaptive filter and output y(n) is produced as close a replica as possible of $N_o(n)$. The filter readjusts its coefficients continuously to minimise the error between $N_o(n)$ and y(n) during this process. Then, the output y(n) is subtracted from the primary input to produce the system output $e = S + N_o - y$, which is filtered signal. The e(n) provides the system control signal and updates the adaptive filter coefficients, which minimises residual noise.

ALE is degenerated form of ANC (Ramli, 2012). ANC has two inputs i.e. primary signal d(n) (signal + noise) and reference signal x(n) (noise) while ALE needs only single sensor and delay to produce a delayed version of d(n), which decorrelates the noise while leaving the target signal component correlated. This is because noise is broadband signal which is not correlated to previous sample values unlike narrowband signal. The delay causes decorrelation between the noise components of input data in two channels while introducing a simple phase difference between sinusoidal components of signal. The adaptive filter responds by forming a transfer function equivalent to that of narrowband filter centred at frequency of narrowband signal. The output y(n) of the adaptive filter in the ALE is an estimate of the noise free input signal. Delay Δ is selected such that Δ is longer than τ_d(BB), i.e., correlation length of broadband noise and smaller than τ_d(NB) correlation length of narrowband signal, beyond these lags, the respective correlations die out quickly, i.e.,

$$\tau_d(\text{BB}) < \text{Delay}(\Delta) < \tau_d(\text{NB}) \tag{1}$$

Development of Adaptive Algorithm is based on Widrow and Hoff's (1960) least mean square (LMS). LMS are class of adaptive filters used to mimic a primary signal d(n) by finding the filter coefficients to produce LMS of error signal e(n).The error signal e(n) is defined as difference between primary signal d(n) and the adaptive filter output. W(n) represents the tap weight of the adaptive filter at the time n. The algorithm starts by assuming a small weight and at each step, by finding the gradient of mean square error (MSE), the weights are updated. The weight equation of LMS is given by:

$$\text{W}(\text{n}+1) = \text{W}(\text{n}) - \mu\text{x}(\text{n})\text{e} \tag{2}$$

x(n) is the input to adaptive filter, μ is the fixed step size. Here negative sign indicates that weights need to be changed in a direction opposite to gradient slope (Vaseghi, 2008).

$$\text{e}(\text{n}) = \text{d}(\text{n}) - \text{W}^{\text{T}}(\text{n})\text{x}(\text{n}) \tag{3}$$

$$0 \le \mu < 2/\lambda_{\max} \tag{4}$$

λ_{max} is the maximum eigenvalue of autocorrelation matrix for the input data x(n).

Maximum convergence is achieved.

$$\mu = 2/(\lambda_{\max} + \lambda_{\min}) \tag{5}$$

λ_{min} is the minimum eigenvalue of autocorrelation matrix for the input data x(n).

With regard to the convergence rate, the variable step size has the better performance than the fixed step of LMS (Vaseghi, 2008). The instantaneous MSE can be minimised through the normalised least mean square (NLMS) algorithm. The step size of NLMS is given as follows.

$$\mu_{NLMS}(n) = 1 / \left[2x^T(n)x(n) \right] \tag{6}$$

The MSE is defined as

$$\xi(n) = E\left[e^2(n) \right] \tag{7}$$

The MSE is a cost function that requires knowledge of the error function e(n) at all time n. For that purpose, the MSE cannot be determined precisely in practice and is commonly approximated by other cost functions. The simpler form to estimate the MSE function is to work with the instantaneous square error (ISE) given by

$$\xi(n) = e^2(n) \tag{8}$$

4 Simulations

Simulations are first done with the synthesised NQR signal and then it is applied to real time NQR signal.

4.1 NQR signal model

NQR signal is often measured as free induction decay (FID) which is response of a atomic nuclei to a single RF excitation pulse. The noise corrupted FID signal is modelled as linear combination of signal S_o with strength A and background noise W_o as shown in equation (9) (Niu et al., 2010).

$$X_o(t) = AS_o(t) + W_o(t) \tag{9}$$

where $X_o(t)$ is NQR response signal, $W_o(t)$ is background noise, which is assumed to be Gaussian random process with mean value zero. The pure FID signal is modelled as,

$$S_o(t) = e^{\frac{-t}{T_2^*}} \cos(2 * pi * fc * t) \tag{10}$$

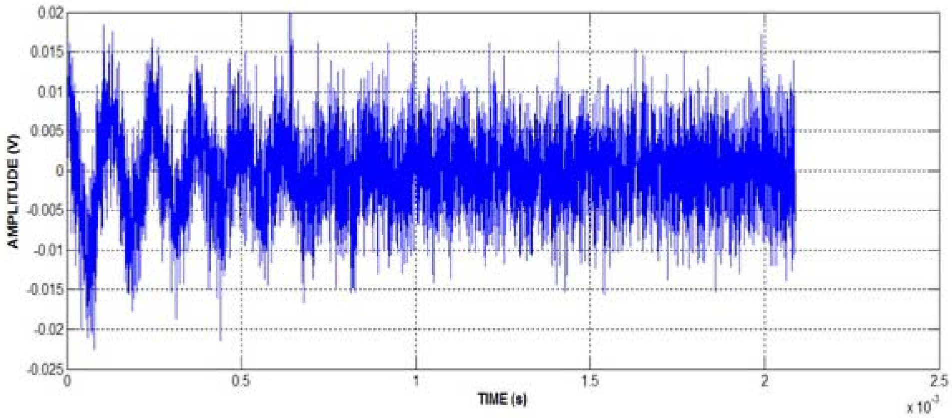
As in the block diagram shown in Figure 1 digital demodulator shown works on lock in amplification technique in which the output is basically the sum and difference of input frequencies from which FIR filter rejects the higher frequencies providing with difference of frequencies. So here in equation (10). T_2^* denote decay time constant and fc denotes difference between FID frequency and reference frequency (assumed to be 8 KHz). The reference frequency is the frequency of RF excitation pulse which may vary slightly from FID frequency. For ^{14}N detection from $NaNO_2$, the decay time constant of FID response with resonance frequency of 4.642 MHz is 0.5 milliseconds (Niu et al., 2010). The amplitude of the FID envelope is assumed to be 10 mV, sampling frequency 2.875 MHz.

4.2 Noise model

NQR background noise includes thermal noises of the coil and external radio frequency interferences (RFI). The power spectrum of the measured noise (from NQR spectrometer) data accumulated and was observed that it is not a white noise. Thus, we can assume that background noise is not white Gaussian noise but coloured noise.

Noise is modelled as white Gaussian noise and then passed through a 30 KHz filter to obtain a bandlimited noise. The simulated noise corrupted NQR signal $X_o(t)$ is shown in Figure 3.

Figure 3 Simulated NQR signal with noise (see online version for colours)



4.3 Adaptive algorithm applied to simulated NQR signal

Simulations for noise reduction are done using normalised LMS block from signal processing blockset of Simulink® of MATLAB. To implement ANC using this block the simulated noise $W_o(t)$ (Reference signal) is given to input port of the block. The noise corrupted NQR signal $X_o(t)$ (Primary signal) is given to the desired input port of the block. Thus the output of the block will give the error and the error signal will give the filtered NQR signal. Wts gives the weights of the filter.

Considering the relationship of sampling rate 2.875 MHz and filter bandwidth , the number of points per period is between 95 and 96, the length of Adaptive filter is M = 256, which is greater than the number of points in two periods (Yang et al., 2010). The step size is calculated by equation (4), i.e., first the eigenvalues of the autocorrelation of the input signal (which is $W_o(t)$ in this case) is calculated and then the step size.

Initial weights are set to zero. When we run the simulation block calculates the filter weights using least mean algorithm. The output port outputs the filtered signal which is the estimate of desired signal which is noise in this case. The error output port outputs the result of subtracting the output from desired signal which is the NQR signal is this case. Figure 4 shows the implementation of ANC in MATLAB.

Figure 4 ANC implemented in Simulink (see online version for colours)

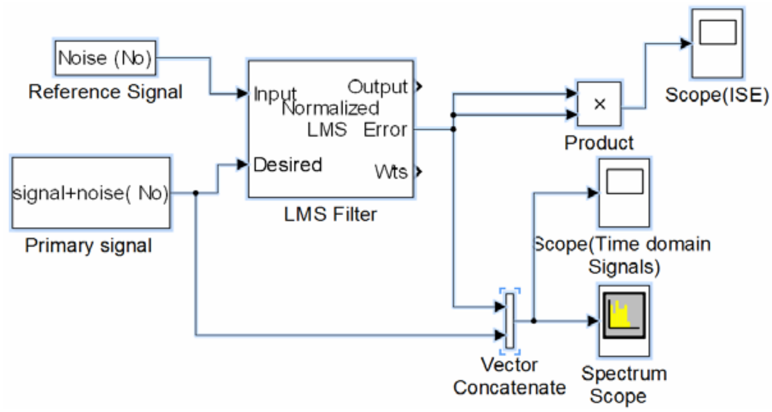


Figure 5 Power spectrum of simulated noise corrupted FID and ANC output (see online version for colours)

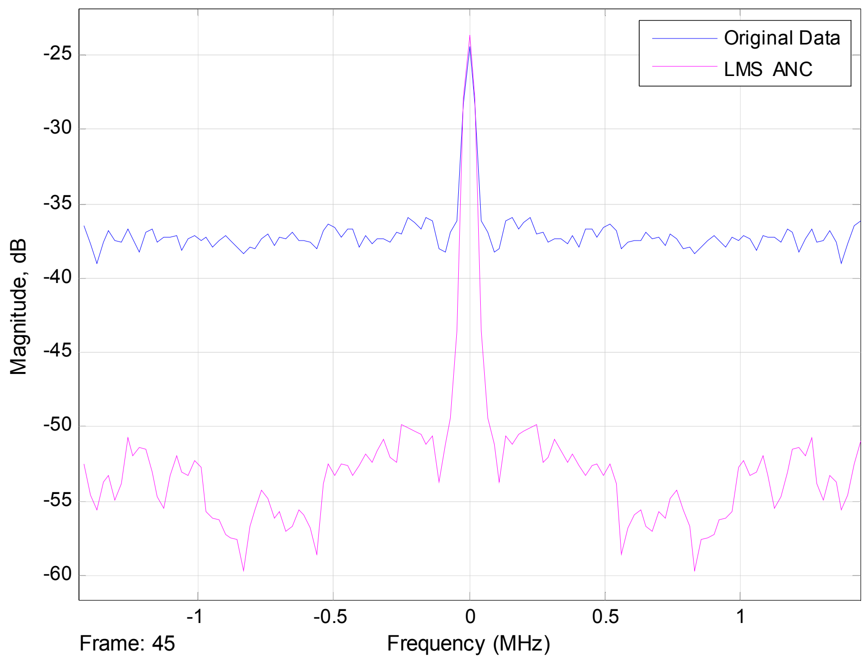


Figure 5 shows the power spectrum of noisy simulated FID and output of ANC. Figure 6 shows the respective time domain signals. Figure 7 shows the ISE for ANC applied to simulated NQR FID and it can be seen that ISE converges in less than 1 millisecond.

Figure 6 Simulated noise corrupted FID and output (see online version for colours)

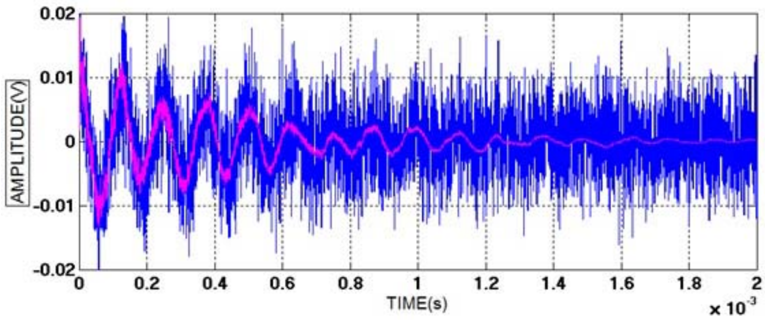


Figure 7 ISE for simulated FID input to ANC (see online version for colours)

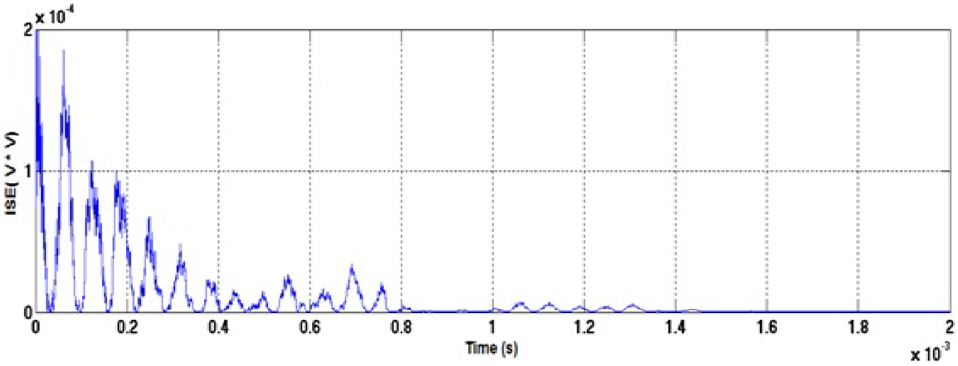
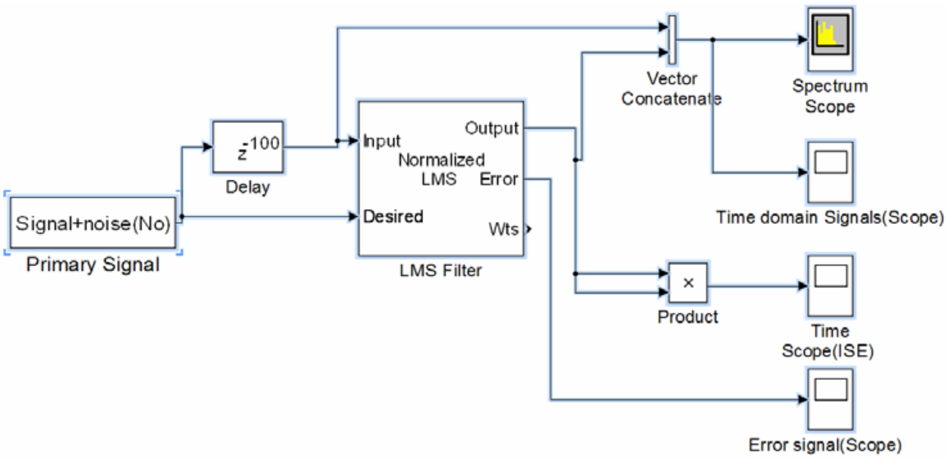


Figure 8 ALE implemented in Simulink (see online version for colours)



The ALE is simulated using LMS block of Simulink® is shown in Figure 8. The reference signal is a delayed version of primary signal so $X_o(t)$ is given to desired port of

LMS block and it is delayed by Δ and given to input port of LMS block of Simulink. NQR signal model $S_o(t)$ is narrowband signal while noise $W_o(t)$ is a broadband signal. The delaying of signal decorrelates the noise component thus the error, i.e., the difference between $X_o(t)$ and ALE output is only noise. The delay is chosen here according to equation (1), i.e., delay $96 < \Delta < 360$ (for NQR signal model as noise bandwidth is 30 KHz and signal is assumed to be 8 KHz, fs/30 = 96, fs/8 = 360).

The other parameters such as length of filter L = 256, step size μ = 0.1 are same as kept for ANC. The error is employed to update the filter weights such that ALE output is close to $S_o(t)$.

Figure 9 shows the spectrum of noisy FID and ALE filtered signals. Figure 10 shows respective time domain signals. Figure 11 shows ISE for ALE applied to simulated NQR FID and it can be seen that ISE converges in 2 milliseconds.

Figure 9 Power spectrum of simulated noise corrupted FID and ALE output (see online version for colours)

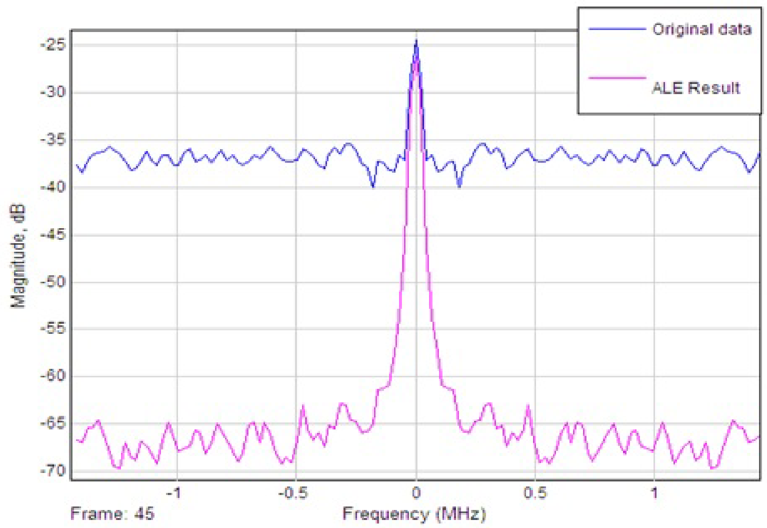


Figure 10 Simulated noise corrupted signal and ALE output (see online version for colours)

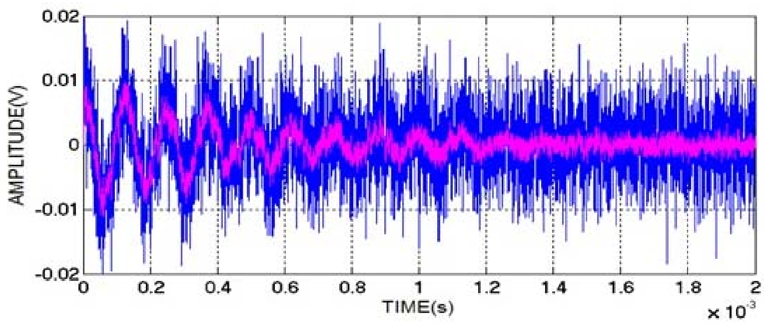
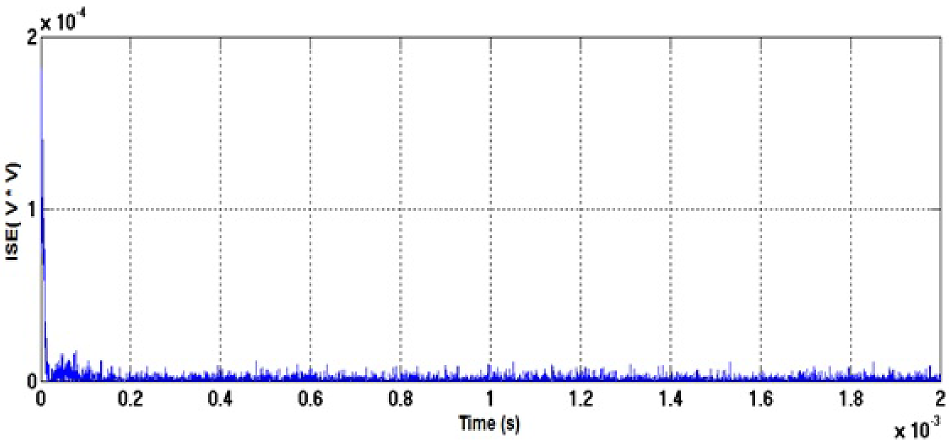


Figure 11 ISE for simulated FID input to ALE (see online version for colours)



4.4 Selection of SNR of input signals for signal model

The steady frequency response of ALE (Wang and Mechefske, 2004) is given as

$$H(\omega) = \frac{SNR}{1 + LSNR} e_o^{-j(\omega-\omega o)\Delta T} \frac{1 - e^{-j(\omega-\omega o)LT}}{1 - e^{-j(\omega-\omega o)T}} \tag{11}$$

$$H(\omega o) = \frac{LSNR}{1 + LSNR} \tag{12}$$

Thus from equation (12), it can be concluded that when SNR of input signal is less than –10 dB, the gain value of the filter tends to be zero thus the filter cannot suppress the broadband noise or enhance narrowband signal. When SNR value is greater than 0 dB i.e., the gain of the filter is greater than one, the narrowband signal will fully pass through the ALE filter and the broadband noise will be suppressed to minimum value according to principle of LMS . Therefore, the input signal of SNR 0 dB is given as input to ANC as well as to ALE.

The performance of the ALE under different parameters such as step size, filter length and SNR has been studied extensively by simulations and experiments. The simulation and experimental results showed that whenever the value of step size is small it leads to good estimation of sinusoidal signal but the convergence speed slows down. On the contrary whenever the value of step size is large, output of ALE becomes distorted and convergence speed increases considerably so the step size is selected midway between the two and is given by equations (5) and (6) for LMS and NLMS respectively.

4.5 Wavelet transform applied to simulated NQR signal

Three steps explained in Section 3.2 are performed on synthesised NQR signal and decomposition of signal is done to level 5 with ‘coif5’ wavelet. The thresholding is done on individual detailed coefficient and finally modified detailed coefficients are added with approximation coefficient to produce filtered signal. In this work Sqtwolog is used for de-noising, in which threshold value is calculated by square root log of length of signal. It is also called as universal thresholding. The filtered signal in time and frequency domain is shown in Figures 12 and 13 respectively. It can be seen that wavelet gives better results as compared to ANC and ALE in case of simulated NQR signals.

Figure 12 Simulated noisy FID and wavelet transform output (see online version for colours)

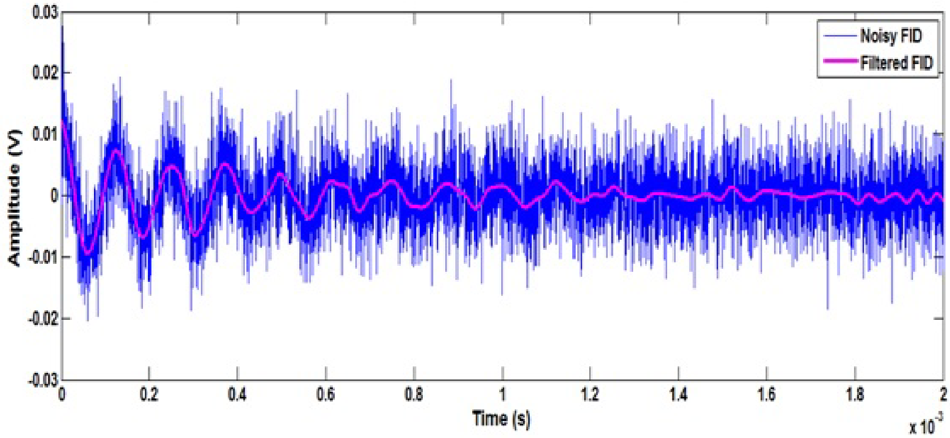
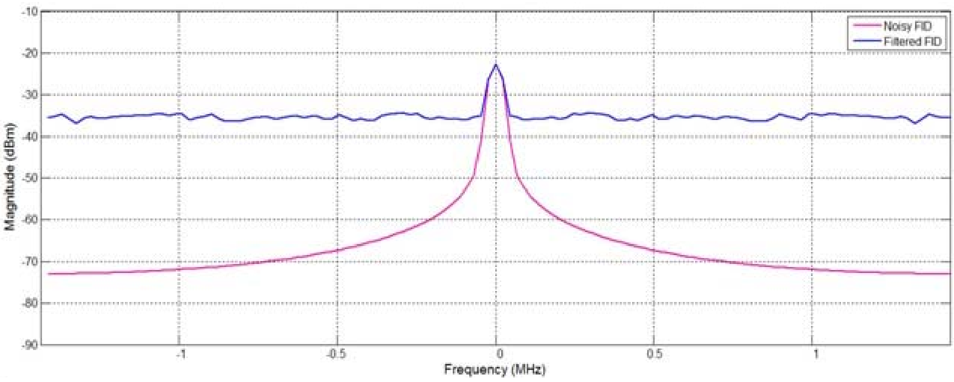


Figure 13 Power spectrum of noisy FID and filtered signal for wavelet transform (see online version for colours)



4.6 Adaptive filtering algorithms and wavelet transform applied to real NQR signal

The real time ^{14}N NQR signal from $NaNO_2$ acquired from NQR spectrometer is shown in Figure 15. Due to low SNR of single FID, it is enhanced by accumulation (Rudakov and Mikhaltsevich, 2003). The results of applying ALE algorithm to real time signal are shown in Figure 15 and the corresponding power spectrum is shown in Figure 14. Figure 16 shows ISE when ALE is applied to real NQR FID signal. The results show that ISE converges within 1 millisecond. The ANC algorithm is not applied to real NQR as noise cannot be acquired separately from NQR signal.

Figure 14 Power spectrum of real time NQR signal and output of ALE (see online version for colours)

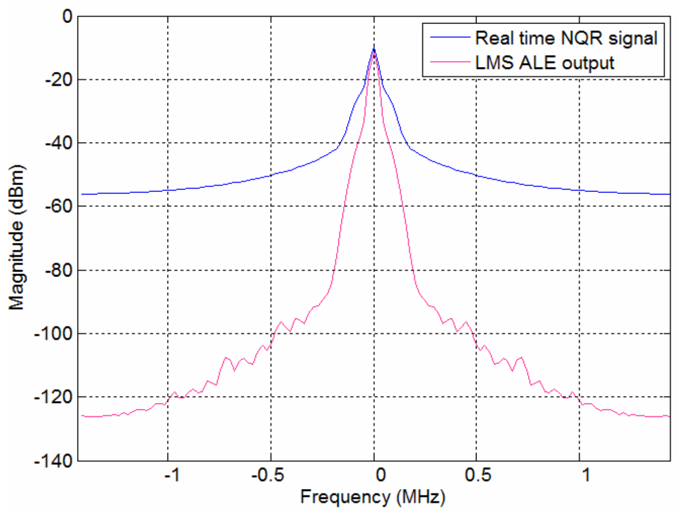


Figure 15 Real time NQR signal at input and output of ALE (see online version for colours)

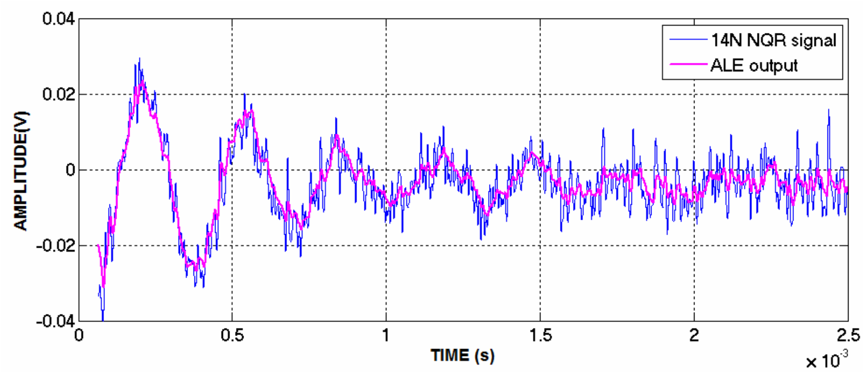
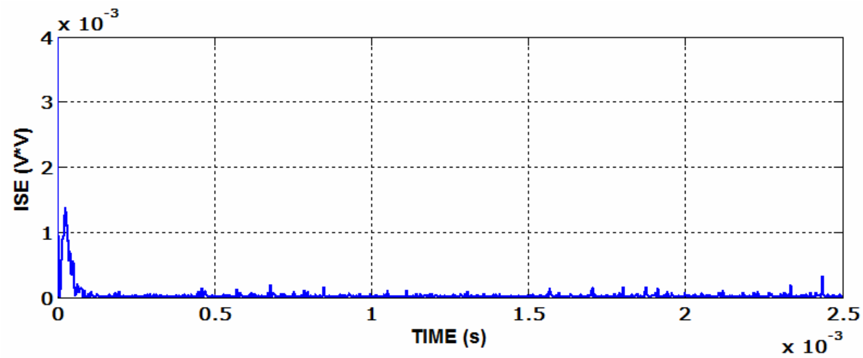


Figure 16 ISE for real time NQR as input to ALE (see online version for colours)



The NQR signal, which is acquired comes through 30 KHz filter so delay for ALE is decided by the cutoff frequency and sampling frequency is 2.875 MHz so delay taken for real time NQR signal is 96 (Ramli, 2012).

Three steps explained in Section 4.4 are performed on real time NQR signal using 'coif5' wavelet. The filtered signal in time and frequency domain is shown in Figures 17 and 18 respectively. It can be seen that ALE gives better results as compared to ANC and wavelet in case of real time NQR signals.

Figure 17 Real time NQR signal and output of wavelet transform (see online version for colours)

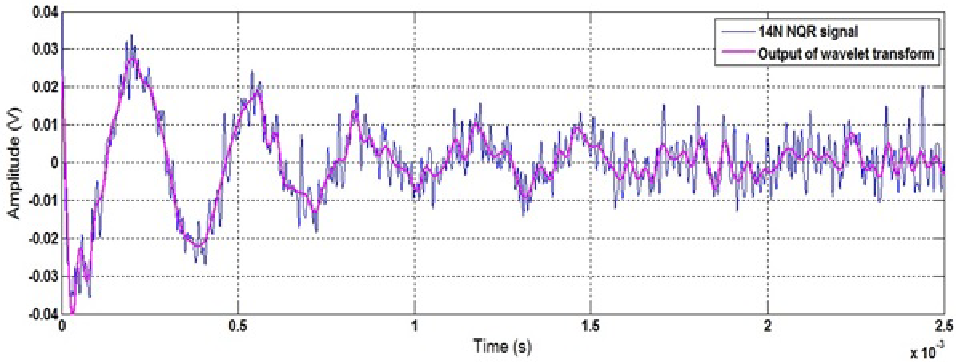


Figure 18 Power spectrum of real time NQR signal and wavelet transform output (see online version for colours)

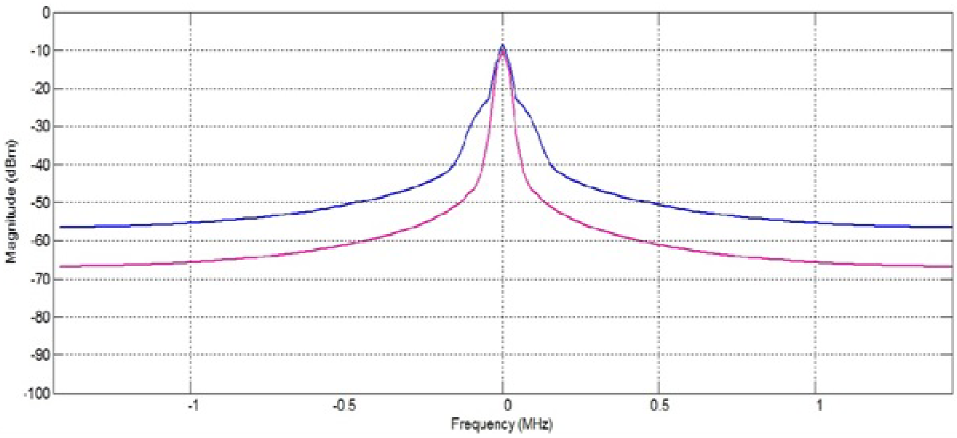


Table 1 shows the effectiveness of various algorithms. It may be deduced that NLMS ALE algorithm score better over other algorithms achieving objective of filtering noisy real time NQR signals.

The SNR increases by $\sqrt{n}$ when the signal is averaged by n times. Thus, a signal which is already averaged by 256 times will increase by 6 dB when it is further averaged by 768 times. Also in our experiment to observe ^{14}N NQR signal form $NaNO_2$ we repeated the pulse after very 0.5 seconds, therefore the time taken by averaging is 6.4 min.

Table 1 Comparison of algorithms

Algorithm	*Noise reduction (approx.)*	*Time*
Simulated NQR data		
NLMS ALE	15 dB	2 msec
NLMS ANC	25 dB	2 msec
Wavelet transform	30dB	
Real NQR data		
Averaging	6 dB	6.4min
NLMS ALE	30 dB	1 msec
Wavelet transform	10 dB	

5 Conclusions and future scope

In this paper, NQR signal processing based on adaptive filters and wavelet transform is presented and it is shown for simulated wavelet transform technique seems to be better as compared to adaptive filtering but for real time ALE is faster and better detection method with improvement in SNR as compared to averaging technique and wavelet transform. Also further incorporating ALE in FPGA is easier as compared to wavelet transform. The NQR spectrometer developed can further be developed in miniature size by combination of RF amplifier, receiver module and FPGA module on one board and thus enhances opportunities for novel and exciting NQR/NMR experiments like explosive detection, mine detection, etc.

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