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A Low-Cost Benchtop NMR System for Measurements of Self-Diffusion Coefficients †

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Abstract

The exponential decay of signals during Nuclear Magnetic Resonance (NMR) experiments results in part from the movement of molecules within the magnetic field gradients present in all real-world systems. For most samples, this motion is driven by molecular self-diffusion. NMR can be used to quantify this important sample parameter, which can reveal the molecular structure of a sample and the interaction of mobile molecules within it. This has a wide range of applications in areas such as the study of porous media, polymer characterization, and quality control in food systems. Most commercial systems that are currently available for diffusion measurements are expensive. This work utilizes a low-cost custom NMR probe system, consisting of a set of permanent magnets, a steel yoke arrangement, and a solenoid transmit-receive coil with custom electronics and a set of magnetic field gradient coils alongside a broadband spectrometer. Using this new system, we show that it is possible to use compact, lower-cost NMR probes to obtain self-diffusion coefficient measurements for two samples: water and 1-pentanol, achieving 3.4×10^{-9} m^2s^{-1} and 4×10^{-10} m^2s^{-1} values for the diffusion coefficients at room temperature (21 °C), compared to literature values of 2.023×10^{-9} m^2s^{-1} at 20 °C and 2.05×10^{-10} m^2s^{-1} at 15 °C, respectively. We thereby demonstrate that such a system allows for self-diffusion coefficient measurements using a pulsed gradient spin echo (PGSE) sequence at a fraction of the cost of typical diffusion measurement instruments.

Keywords: magnetic resonance relaxometry; low cost; benchtop; self-diffusion measurements

1. Introduction

Nuclear magnetic resonance (NMR) is a useful technique for investigating molecular dynamics. Among its many applications, NMR can be used to measure molecular self-diffusion, which is a process that arises from the random Brownian motion of molecules in a fluid. This net collective motion is defined by the self-diffusion coefficient, D [1].

Measurements of the diffusion coefficient can be achieved through the application of magnetic field gradients. The position of NMR-active molecules within this gradient is encoded into the NMR signal. If molecular motion occurs before the application of an opposite decoding gradient, there will be attenuation of the signal. This is directly linked to the extent of molecular displacement and can therefore be used to determine D [2].

Pulse Field Gradient (PFG) NMR utilizes magnetic field gradient pulses that are applied for short, well-defined periods of time. Varying the strength and duration of these pulses allows for diffusion measurements to be tailored to the system under investigation.

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A key PFG experiment, first demonstrated by Stejskal and Tanner in 1965 [3], is the Pulsed Gradient Spin Echo (PGSE) sequence. This experiment is based on a conventional spin-echo NMR sequence, which consists of a 90° radio frequency (RF) pulse followed by a 180° pulse. The 90° RF pulse is used to generate the NMR signal, and the 180° RF pulse stores signal coherence that would otherwise be lost, producing a detectable signal.

Two gradient pulses are then incorporated into this sequence to allow diffusion measurements. The initial gradient pulse effectively labels the position of the molecules within the sample, whereas a second gradient pulse attempts to reverse this labeling after a defined diffusion period. For molecules that have remained stationary, the second gradient pulse cancels out the effect of the first, whilst molecules that have undergone diffusion will not. This results in a reduction in the measured NMR signal intensity. An example of this sequence can be seen in Figure 1.

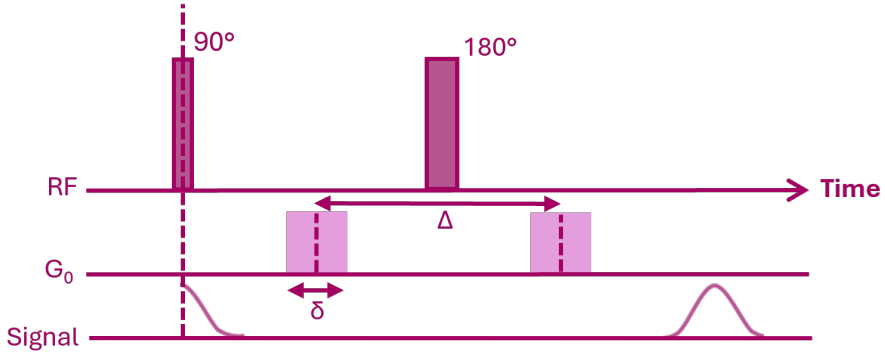


Figure 1. An example of a PGSE sequence, showing the RF pulses, gradient pulses, and resulting signals.

The normalized signal attenuation can be related to D via the following equation referred to as the Stejskal–Tanner equation:

$$\ln\left(\frac{S}{S_0}\right) = -\gamma^2 G_0^2 \delta^2 \left(\Delta - \frac{\delta}{3}\right) D \quad (1)$$

where δ is the duration for which the pulsed gradients are switched on, and Δ is the time for the molecular diffusion to take effect. D is measured by obtaining several measurements with varying gradient strengths. The resulting normalized signal attenuations can then be plotted according to Equation (1) to determine a value for D.

However, the Stejskal–Tanner equation assumes a perfect square gradient pulse. For non-ideal pulse shapes, a generalized equation utilizing the integral of the gradient pulse waveform is required [4]. This is given by:

$$\ln\left(\frac{S}{S_0}\right) = -\gamma^2 D \left(\Delta - \frac{\delta}{3}\right) \int G(t) dt \quad (2)$$

2. Materials and Methods

An NMR probe was constructed using two N52 neodymium permanent magnets (First4Magnets, Tuxford, UK) in a custom housing unit. Steel yokes and shaped pole pieces were added into the design to redirect the stray magnetic field produced by the permanent magnets and improve the magnetic field homogeneity in the region where the sample would be positioned. Field homogeneity is an important requirement for NMR experiments, as variations in this static magnetic field can reduce measurement sensitivity.

Custom RF electronics were developed for transmitting and receiving signals. These electronics were connected to a single transmit-receive RF coil containing the sample. During an experiment, the RF coil delivers short RF pulses to excite nuclear spins and then subsequently detects the NMR signals produced as the spins relax and rephase.

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These custom electronics consisted primarily of tuning and matching circuitry that was critical to the performance of the probe. Due to differences in the coil geometry and electrical characteristics compared to coils used in commercial systems, custom circuitry is necessary for bespoke probe designs. It provides the flexibility needed to accommodate these variations in the coil to ensure that it is correctly impedance-matched to the transmitter and receiver. This maximized the transfer of the induced NMR signal to the receiver and minimized losses caused by impedance mismatches. As a result, this improved the signal-to-noise ratio (SNR) and enabled the detection of weaker signals and enhanced overall measurement sensitivity.

Diffusion measurements using this system were then enabled through the addition of two magnetic field gradient coils. These coils each comprised 10 turns of 0.4 mm enameled copper wire wound in opposite directions, much like an anti-Helmholtz coil, on an acrylic support bobbin. When driven with current, this produced a linear magnetic field gradient across the sample volume.

These gradient coils were then oriented with the field perpendicular to the RF coil and secured to the custom tuning and matching Printed Circuit Board (PCB). This maintained the alignment of the coils relative to the RF coil and sample and minimized movement throughout the experiment. The full assembly of this PCB can be seen in Figure 2.

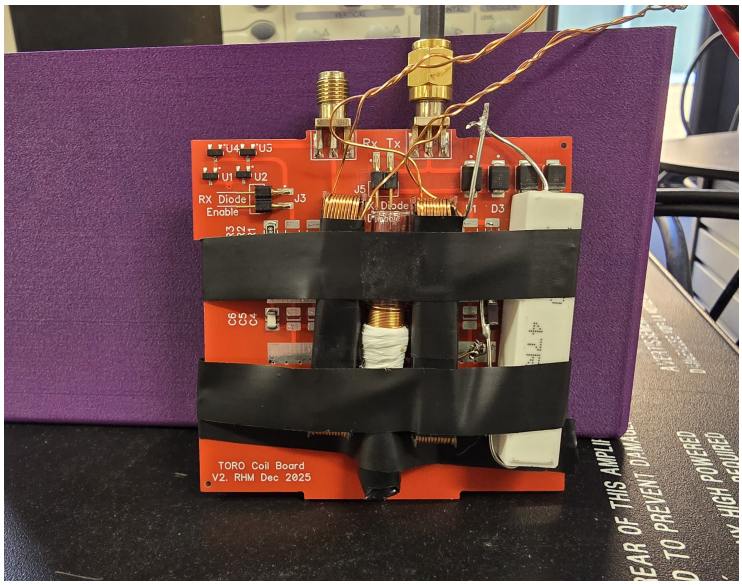


Figure 2. Gradient coils positioned on the tuning and matching board parallel to the coil and sample.

Gradient pulses were generated by an NMR spectrometer (Kea^2, Magritek, Wellington, New Zealand) and were then amplified using a power amplifier (LVC 5050, Techron, IN, USA). This was then applied to the gradient coils to produce the pulsed magnetic field gradients.

Testing and Validation

Table 1 shows two samples with known diffusion coefficient values which were used to test the system [5].

A standard PGSE sequence was used to measure the diffusion coefficients of distilled water and 1-pentanol at room temperature (21 °C). The scan parameters for these experiments can be seen in Table 2.

To account for deviations from the idealized rectangular gradient pulse assumed by the Stejskal–Tanner equation (Equation (1)), the actual gradient waveform generated by the system was measured and incorporated into the modified form, given by Equation (2). The

waveform corresponding to each gradient pulse was recorded using a digital storage oscilloscope, and its time integral was calculated and used to calculate the diffusion coefficient.

Table 1. Diffusion coefficient values for distilled water and 1-pentanol at given temperatures.

Sample	Diffusion Coefficient (m^2/s)	Temperature (°C)
Distilled water	2.023×10^{-9}	20
1-Pentanol	2.05×10^{-10}	15

Table 2. Scan parameters for PGSE experiment for distilled water and 1-pentanol.

Parameter	Value
Δ	2000 ms
δ	1000 ms
Pulse length	2.4 µs
Gradient	0–0.5 T/m

3. Results

The results obtained for distilled water are shown in Figure 3. The time integral of the gradient pulses was plotted against the normalized signal. The slope of the linear fit was used to calculate the diffusion coefficient by

$$D = -\frac{slope}{\Delta - \frac{\delta}{3}} \quad (3)$$

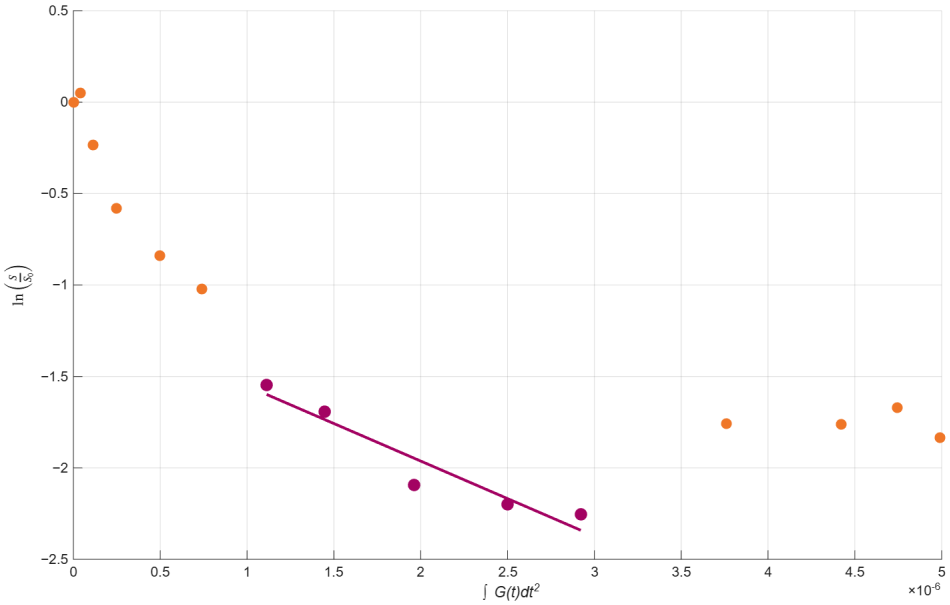


Figure 3. Full PGSE results for distilled water, with the points contributing to the diffusion coefficient calculation and associate fit highlighted in purple.

Several data points were excluded from the fit due to significant deviations from the overall trend. Fitting the remaining data points yielded a diffusion coefficient of $(3.4 \times 10^{-9} \pm 6 \times 10^{-10})$ m^2s^{-1}.

The results obtained for 1-pentanol are shown in Figure 4. As with the distilled water, some points were omitted from the fitting procedure due to poor agreement with the overall trend. Analysis of the remaining data points yielded a D value of $(4 \times 10^{-10} \pm 1 \times 10^{-10})$ m^2s^{-1}.

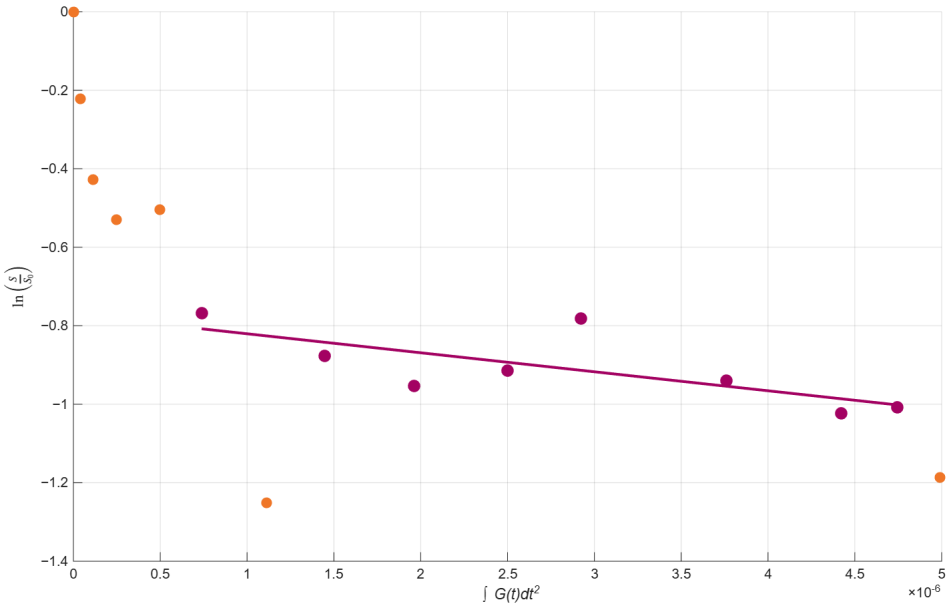


Figure 4. Full PGSE pentanol results, with the points contributing to the diffusion coefficient calculation and associate fit highlighted in purple.

4. Discussion

The measured diffusion coefficients for both distilled water and 1-pentanol were in reasonable agreement with literature values within the calculated uncertainties. However, several issues were encountered during data processing. For both samples, the initial data points exhibited significant deviations from the overall trend and were therefore excluded from the analysis. In addition, several data points corresponding to larger gradient time-integral values in the distilled water dataset were removed due to their poor agreement with the expected behaviour.

The deviation of these high-gradient data points is likely due to the NMR signal becoming heavily attenuated at large diffusion weightings. As the signal approaches the background noise level, the measurements become less reliable. These points were therefore considered unsuitable for inclusion in the fitting procedure, as they would have a negative impact on the accuracy of the calculated diffusion coefficient.

A number of factors may have contributed to these deviations, such as relatively poor signal-to-noise ratio (SNR), which may have reduced the reliability of the normalized signal attenuation values. Inclusion of these anomalous points results in poor-quality fits and D values that were not representative of the overall trends and they were therefore excluded from analysis. The removal of these points resulted in linear fits that more accurately reflected the diffusive behaviour of the samples and yielded diffusion coefficients that were in reasonable agreement with literature values.

The rapid switching of the gradient field also generates eddy currents which can distort the gradient waveform and produce residual magnetic fields that persist after the nominal gradient pulse has ended. This can alter the effective diffusion weighting and introduce additional signal attenuation. By measuring the actual gradient waveform and incorporating it directly into the modified Stejskal–Tanner equation, the influence of these distortions can be reduced but is not completely removed and likely still has some impact on the overall signal attenuation.

Temperature fluctuations were also identified as a significant limitation. Variations in the laboratory temperature, in addition to potential heating of the coils and electronic components over extended operation, may have altered the temperature of both the sample and the measurement conditions over the duration of the experiment. Whilst some experi-

mental parameters were adjusted to try and compensate for these changes, this also resulted in the inclusion of additional background noise that potentially reduced the accuracy of the diffusion measurements and resulted in the observed anomalous points.

The size of the samples used for this experiment also likely had a negative impact on the results. Due to their small size, the proximity of the sample to the walls of the NMR sample tube may have influenced the measured diffusion behaviour and potentially introduced boundary effects that are not typically observed in diffusion experiments with larger sample volumes. These effects may have introduced additional uncertainties into the measured values for the diffusion coefficient.

Despite these limitations, these results demonstrate the feasibility of performing diffusion NMR measurements using this low-cost system. The measured diffusion coefficients showed good agreement with literature values, providing confidence in the overall approach. Future work should focus on improving temperature stability, increased sample size capabilities, and reduction in background noise. These improvements would further strengthen the potential of this system as an accessible and cost-effective platform for diffusion NMR experiments.

5. Conclusions

This work has demonstrated the feasibility of performing diffusion NMR measurements using a low-cost permanent-magnet NMR probe equipped with custom pulsed field gradient capabilities.

Diffusion measurements were successfully acquired for distilled water and 1-pentanol, with the calculated self-diffusion coefficients showing reasonable agreement with the literature values within the associated experimental uncertainties. These results indicate that the developed probe is capable of producing reliable diffusion measurements despite its relatively simple and cost-effective design. The successful determination of diffusion coefficients demonstrates the effectiveness of the gradient coil assembly and confirms the suitability of the system for diffusion NMR investigations.

Overall, the results demonstrate that accurate diffusion measurements can be achieved using a compact permanent-magnet NMR system. Future work should focus on improving temperature control, reducing background noise, reducing the effect of eddy currents, optimizing gradient coil performance, and increasing sample volume capacity. Such developments would improve measurement accuracy and robustness, further enhancing the potential of low-cost permanent-magnet systems as accessible platforms for diffusion NMR research and applications.

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Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

NMR	Nuclear magnetic resonance
PCB	Printed circuit board
PFG	Pulsed field gradient
PGSE	Pulsed-gradient spin echo
RF	Radiofrequency
SNR	Signal-to-noise ratio

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