Shortening NMR diffusion experimental times

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NMR diffusion measurements have become the method of choice for measuring diffusing due to their wide applicability, speed of measurement, enormous range of accessible diffusion coefficients (from gas ~10^{-6} m^2s^{-1} to large polymers ~10^{-15} m^2s^{-1}), and the ability to measure diffusion over a specified timescale, Δ, which greatly adds to the power of NMR diffusion measurements as it allows the ability to probe porous media [1,2]. The weakness of NMR diffusion measurements lies in their inherent insensitivity. Consequently, many experiments are in theory possible but in practice would simply consume too much spectrometer time and therefore become impractical. Even in cases where the total measurement time is not a limitation, making the measurement faster expands the horizons of diffusion measurements to study reaction kinetics [3,4], as well as simply increasing throughput.

We have been developing new approaches for increasing the speed of NMR diffusion measurements with particular emphasis on generally applicable techniques that are both simple yet do not come at the cost of reduced information (e.g., loss of chemical shift information or loss of the specified diffusion measurement timescale, Δ).

Here we demonstrate that it is possible to shorten NMR diffusion measurements by more than 70% without any loss in accuracy by a trivial change in the experimental acquisition procedure. Specifically, NMR diffusion measurements are typically run as an arrayed experiment in which a particular gradient value, *g* (i.e., the arrayed variable) is chosen and the experiment is repeated for a set number of scans (*NS*). The arrayed variable is then incremented and a signal acquired averaged over *NS*. This procedure is typically repeated for something like 15 gradient values in total. Conventionally, NMR diffusion measurements are performed with the same *NS* at each iteration of the experimental parameter despite the SNR being more than sufficient for many of the iterations. However, enormous time saving can be found by varying *NS* as a function of the experimental parameter (i.e., *g* in this case) and the signal normalised by the number of scans used at each iteration [5]. Hence, this **new normalisation approach** requires far fewer total scans. The method can even be combined with other techniques to increase efficiency [6,7].

References

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