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Comment on mr-2021-56

Anonymous Referee #2

Referee comment on "Selective excitation enables encoding and measurement of multiple diffusion parameters in a single experiment" by Neil MacKinnon et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-56-RC2, 2021

In this article, MacKinnon et al. describe a pulse sequence that makes it possible to use different diffusion-encoding parameters for different resonances in a single experiment. To achieve this, they replace all the hard pulses of a stimulated-echo sequence by selective ones, except for the final 90° pulse, and they introduce a loop for the dephasing and rephasing blocks. They illustrate the results on a sample consisting of a tri-peptide in H2O:D2O. The pulse sequence may be relevant for the analysis of samples that have components with widely different diffusion coefficients. In its present form, however, the manuscript does not provide sufficient information to show or explain the benefits of the new sequence. I recommend that it be reconsidered after major revisions.

The exact benefit of using different gradient ramps for the different resonances should be clarified. Is it expected to improve the precision of the measured diffusion coefficient? The trueness? Both? This is hard to understand in the present manuscript. Maybe the authors should report the uncertainty of the fit for the selective and non-selective experiments? Also, in Table 1, the value of the diffusion coefficient for water measured with the selective experiment is further way from the calibration value that than measured with the non-selective experiment. Please explain if that it an improvement, and why?

Why does SNR increase in the selective experiment for the MAS signal? Is that a positive observation? Or is that a reflection of the fact that coherence transfer pathway selection is not as effective?

Please provide the values of the encoding gradient in G/cm or T/m, or the maximum gradient that can be delivered by the probe. These probes typically deliver up to 200 or 300 G/cm. Together with the diffusion delay of 250 ms and a ramp of up to 95%, this would results in an unusually strong attenuation. Please clarify.

The authors state that the experiment is accelerated by a factor of n. In the example that they report, n = 3 but two of the resonances belong to the same molecule, and are encoded with the same parameters. So, isn't the acceleration by a factor of 2 only?

More generally, stating that the experiment is accelerate will only be valid once the authors convincingly explain why there is an advantage of using different ramps.

The author state that the approach is applicable to any diffusion experiment. This is not obvious, in particular for spin echo based experiment. Once one of the resonances is in the transverse plane, it experiences any subsequent gradient pulse. How would it work to encode independently the different resonances ?

It would help to discuss examples where one would want to use this pulse sequence. If the gradient ramp are tailored for the selected resonances, it means that the corresponding diffusion coefficients are know at least approximately. So what would the accelerated experiment be used for? The introduction covers a broad range of applications of diffusion NMR, but no connection is made, in the discussion, between these area of application and the proposed method. For example, the abstract states the possibility to encode multiple delay or multiple directions; does that assume that several resonances are available for the same molecule?

Two minor points:

It would be helpful to also show the pulse sequence without the loop structure, that is, the complete pulse sequence with a fixed value of n. Please also indicate, in this figure, the exact definition of Delta. This would help the reader to see that the Delta delay is the same for all of the selected resonances.

Why use two different steps to encode the two MAS resonances, rather than a single one using a dual-band selective pulse?