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Discussions

Interactive comment on "RIDER distortions in the CODEX experiments" *by* Alexey Krushelnitsky and Kay Saalwächter

Anonymous Referee #2

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The main focus of this article is to trace the origins of the unexpected decay seen in the CODEX dephasing profiles due to the RIDER effect, even when no motion is present in the sample. The authors conclusively show that even when utmost care is taken, the RIDER effect can dominate the decay during the CSA-CODEX mixing time, especially if the antiphase component is not suppressed. The authors clearly demonstrate the features in their experimental datasets that can be used to verify whether the RIDER effect is in play (the difference in the Sinf/S0 ratio of the in-phase and anti-phase component). They further go on to show that the fast-decaying component in GB1 and SH3 is clearly due to the RIDER rather than motion induced CODEX dephasing. Additionally, the RIDER effect in deutarated samples due to 2H-15N dipolar coupling is characterised as well. They go on to suggest a (partial) solution to this problem: the

application of a Z-filter to remove the antiphase component just after CP.

Major comments

The authors have proposed the addition of a Z-filter just after the CP to remove this effect. However, as seen from Fig 7. this does not seem to work at all for the antiphase term in CSA CODEX (which is where one should see a prominent effect). Similarly, for carbonyl, the use of Z-filter is not sufficient to remove these artefacts completely (Fig 9). The final conclusion also seems to be to use only the in-phase component which is less susceptible to this effect, and I would contend that this is the more important of the two. In this light, the abstract, and several statements in the main manuscript appear to me to be misleading when they suggest that the Z-filter takes care of this distortions. Wouldn't something like "Z-mixing and the use of the in-phase component alone" be more appropriate (similar to the final conclusions)

Except in the Fig 12 caption, it is not made clear that only the in-phase component is used for the CODEX data on proteins. I recommend that this be explicitly made clear in the main text.

No pulse is used on 1H during the Z-filter. Will CW decoupling during this period help?

It is unclear what the mechanism for RIDER distortions in the in-phase signal for the CSA-CODEX experiment are (Fig 7, COS component). Is this attributable to imperfect decoupling during the CSA recoupling element?

The conclusions of this article are contrary to the authors' 2009 article on the same subject. This is not clearly bought out, I think it will be very important for the NMR community that this be pointed out clearly and discussed clearly in the manuscript, somewhere near Lines 405-415 (where this is partially done).

Minor Comments

The authors have previously stated (Reichert and Krushelnitsky 2018) that the in-phase component cannot be selected out in a CSA-CODEX experiment. Can this be clarified

in light of Fig. 3?

L 215: "...instability of the MAS controller". How much is this instability, and presumably the rotor synchronization of the pulse sequence by monitoring the output of the mas controller should take care of this?

L 215-220: Does the five-point filter mean that each point shown in the figures is a average of five points, 2 before and 2 after the plotted point? Is this used only for visualisation or for fitting as well?