

Magn. Reson. Discuss., referee comment RC1
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Comment on mr-2021-64

Anonymous Referee #1

Referee comment on "Correction of field instabilities in biomolecular solid-state NMR by simultaneous acquisition of a frequency reference" by Václav Římal et al., Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2021-64-RC1>, 2021

[Overview]

The authors present the SAFR method for collecting a single calibration FID prior to collecting each scan in an experiment for the purpose of correcting chemical shift errors resulting from field instabilities. The method can handle errors resulting from natural drift, temperature fluctuations, cryo fills, and even hardware failures. The theory of the SAFR method is presented and several compelling example applications are shown. The paper is well-written and the method would be of interest to the community.

[Specific Comments and Questions]

In 70 - The introduction acknowledges other simultaneous acquisition schemes, but a discussion of these existing approaches should be included. What is SAFR contributing that improves on what is already available?

In 75 - I thought Eq 1 was clear in how it uses t_{acq} , but the sentence that follows introduces relationships with t_{dir} , t_1 , and t_2 in various cases. I assume t_{acq} is the time coordinate along the FID acquisition, and maybe t_{dir} is the total time it takes to collect a FID? You need explicit definitions in this section.

In 125 - There seems to be a gap between the theory and the application. The theory derives a rotation matrix (and its inverse) that accommodates different rotations for the real and imaginary components, but the paper does not illustrate or completely explain how the SAFR spectra are processed so that the corrections may be applied.

In 255 - The drift is clearly corrected, but how robust is SAFR in recovering peak shapes / peak volumes? The uncorrected peaks in the 4 spectra in Figure 5B show incorrect positions, but each has a correct peak shape. The variation in position makes the "summed" representation in the last row appear to have broadening along 1H. Discussing this or quantifying this would be a nice addition.

In 266 - The delay time between scans along the indirect dimension of the outermost loop will be much longer than between scans along inner loop dimensions. While SAFR appears to work great, is there some additional benefit that could result from either optimizing the order of the indirect dimensions or running multiple experiments and varying the dimension order in each (in all cases, using the same total number of transients as the original)?

[Minor Comments]

In 63 - "Our work presented here extends the linear drift compensation (Najbauer and Andreas, 2019) for a general non-linear case." You may be underselling yourself. In addition to handling nonlinear drift, you are also handling discontinuities that arise from things like the helium fill shown in Fig 5C.

In 130 - Fig 1 is a very nice visual aid. I found it slightly distracting that the arc segments depicting both rotations and all dashed lines "overshoot" what they are labeling.

In 345 - The statement of code availability is fine, but why is the data only "upon request?" Can the data be deposited with the code?