MAGNETIC RESONANCE
Discussions

Magn. Reson. Discuss., referee comment RC3
https://doi.org/10.5194/mr-2021-43-RC3, 2021

Comment on mr-2021-43

Anonymous Referee #2

Referee comment on "Effects of radial radio-frequency field inhomogeneity on MAS solid-state NMR experiments" by Kathrin Aebischer et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-43-RC3, 2021

Reviewer comment: Aebischer et al. 2021

This very good paper characterizes the effect of radial rf field inhomogeneity on MAS solid-state NMR experiments in great detail, both in simulations and experimentally. This type of inhomogeneity leads to rotor-periodic amplitude and phase modulations within the sample under magic angle spinning. The authors could demonstrate that this does not have a significant effect on a number of commonly used experiments. They present their findings in a clear and very detailed manner.

Nevertheless, I still would like to propose some improvements:

First, in the section on nutation experiments, the authors attribute the lower intensity of the sidebands caused by amplitude modulations (compared to the phase modulation sidebands) partially to the lower magnitude of the amplitude modulations themselves. However, the magnitudes of both modulations do not seem too different when looking at Fig. 2 and taking the different scales of amplitude and phase into account. The second explanation provided by the authors (the broadening of the sideband by axial rf inhomogeneity) seems more likely. This could be tested in a simulation that only includes the radial amplitude modulation and not the axial inhomogeneity profile, which would remove the broadening of the sideband.

Second, in the section on cross-polarization, the difference of the rf field inhomogeneity of the two rf fields across the sample is held responsible for the restriction of the active sample volume. But the rf fields on the two channels do not need to have different rf profiles, the mere existence of rf inhomogeneity is sufficient to make the matching condition in Eq. 37 impossible to attain within the whole sample at the same time.

Furthermore, I want to suggest several changes to figures:

Fig. 2 may benefit from two changes. The first would put the panels showing z = +4 mm and z = -4 mm on the same vertical scales (they are very similar already, but not the same). The second would add another set of panels showing the largest radius of each axial position on the same scale to illustrate the difference in magnitude along the rotor axis.

In Fig. 3, vertical scales would be especially useful on the insets showing the sidebands caused by amplitude modulation, since they are barely visible in the main graphs, making an estimation of the scale all but impossible.

The meaning of the arrows in Fig. 11 is described in section 4.2, but not in the figure caption, where I was first looking to find out what they meant.

In addition, there are a small number technical errors that caught my eye:

- The paper by Tošner et al. from 2017 does not include any actual optimal control calculations, as suggested by the citation in line 43 (their tm-SPICE pulses were presented in 2018).
- The insets in panels b) and d) of Fig. 3 look exactly the same despite the relevant parts of the main graphs looking different, has there been an accidental duplication?
- In line 437, Fig. 9c/d is referenced, but the authors likely mean to reference Fig. 9e/f.
- The first sentence of the caption to Fig. 9 makes it look like the simulations for all panels were done at 150 MHz, which, according to the text and a later sentence in the same caption, is not the case.
- In the last sentence of the caption to Fig. 10, the line splitting is placed in panel d) instead of c), and it can *be* attributed.
- “NRM” in line 583 is probably supposed to read “NMR”.