

Magn. Reson. Discuss., author comment AC3 https://doi.org/10.5194/mr-2021-43-AC3, 2021 © Author(s) 2021. This work is distributed under the Creative Commons Attribution 4.0 License.

Reply on RC3

Kathrin Aebischer et al.

Author 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-AC3, 2021

We would like to thank the reviewer for the very careful reading of the manuscript and the useful suggestions to improve the presentation.

Q: 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.

A: We have looked into this in a bit more detail and this is correct. We have deleted the sentence on line 277: "The reduced intensity of these amplitude-modulation sidebands can be explained by the lower magnitude of amplitude modulations in comparison to phase modulations (see Fig. 2)." The reason is really the distribution of the sidebands over a larger spectral range which we have also confirmed in simulations as suggested by the reviewer.

Q: 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.

A: We agree with the reviewer that the presence of rf-field inhomogeneity alone will lead to a mismatch in parts of the probe. We have rephrased the relevant text after EQ. (37) to: "Due to the rf-field inhomogeneity across the sample, this condition cannot be fulfilled simultaneously in the entire sample volume and only certain parts of the sample will participate in the polarization transfer thus decreasing the resulting signal intensity."

Q: 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.

A: We have adjusted the scaling of the two panels in Fig.2 but we have not added a separate panel with the largest radius. The reason for this is that the figure would become too small to recognise any details. In addition, the shape of the rf inhomogeneity is not something that we investigated but only copied and used from previous work.

Q: 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.

A: We agree that this is a good idea and have added the vertical axis to the insets.

Q: 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.

A: We have added a sentence to the figure caption that explains the meaning of the arrows: "The arrows indicate the positions of the carrier frequency."

Q: 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).

A: We have corrected the citation for the Tosner 2017 and 2018 papers.

Q: 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?

A: There was indeed a mixup and one of the insets was duplicated and wrong. Thanks a lot for spotting this. It has been updated in the revised version of the manuscript.

Q: In line 437, Fig. 9c/d is referenced, but the authors likely mean to reference Fig. 9e/f.

A: corrected

Q: 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.

A: corrected

Q: 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.

A: corrected

Q: "NRM" in line 583 is probably supposed to read "NMR".

A: corrected