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Magn. Reson. Discuss., referee comment RC2
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Comment on mr-2021-14

Paul Vasos (Referee)

Referee comment on "Extended Bloch–McConnell equations for mechanistic analysis of hyperpolarized ^{13}C magnetic resonance experiments on enzyme systems" by Thomas R. Eykyn et al., Magn. Reson. Discuss., https://doi.org/10.5194/mr-2021-14-RC2, 2021

In terms of scientific impact, discussions (and re-discussions) of the kinetics of hyperpolarised magnetisation

in presence of chemical exchange and relaxation should be of interest to the community. The paper attempts

to clarify two questions that are glossed over in many dissolution-DNP papers: i) substrate-enzyme binding effect

on the relaxation rate constants of the substrate and ii) alteration of the kinetics of isotope-labelled product polarisation

by an unlabelled pool substrate or product. Even if the paper were not entirely original, the thorough discussion

of these topics makes it worth reading.

Could the equations be presented as Polarisation(time)*Substrate_Concentration(time) ?

This way, two variables that obey to different kinetic rate constants could be separated.

In terms of presentation, the paper would gain by exploring some cases such as R_1>> k_1,-1

R_1<<k_1,-1, passage through a membrane before enzymatic conversion, or high enzyme concentrations.

In the latter case, equations seem to predict an abrupt decrease of product magnetisation levels,

a discussion would be welcome.

References are not complete, at least papers where experimental data was acquired on the kinetics of

substrates used as examples in this article should be cited.

Minor aspects:

lines 282-287: if k_-1 = k_-1, is the equilibrium value M_z,eq,A/M_z,eq,B = 1/0.8 ?

Figure 8: Equations in (a) appear truncated.

Necessary improvements:

Supporting material containing the Matlab program with appropriate comments should be made

available to the readers.