Bloch-McConnell Simulation Study – Comparison of 14 Frameworks

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INTRODUCTION: Quantitative CEST (qCEST) approaches can provide access to solute exchange rates and concentrations by using the underlying Bloch-McConnell (BMC) equations[1,2]. Previously, we compared BMC simulation frameworks from several research groups for simple continuous wave saturation cases and were able to reduce initial deviations between them significantly[3]. This work extends the comparison to pulsed saturation with shaped RF pulses, aiming to establish a community-approved validation for pulsed CEST simulations.

METHODS: All necessary simulation settings and information were provided on our public GitHub repository[4]. In total, 4 new simulation cases covering different pulsed saturation schemes with shaped and rectangular RF pulses and two different pool models were defined. All participants submitted their simulation results to an online spreadsheet.

RESULTS: The simulation results for the 4 new cases (numbered 5 to 8) from all 14 participating CEST groups/simulation frameworks are shown in Figure 1. After several adaptions, the results #1-5, #8-10, #13 and #14 show a good match across all new cases. For case 5 (Fig. 1A, single Gaussian pulse), results #6, #7, #11 and #12 deviate from the main cluster and from each other. Similarly, in case 6, which involves a pulse train of the shaped pulse from case 5, these deviations persist. In case 7 (Fig. 1C, same pulse train in a 5-pool system), only result #11 shows essential deviations. All results for case 8 show adequate agreement.

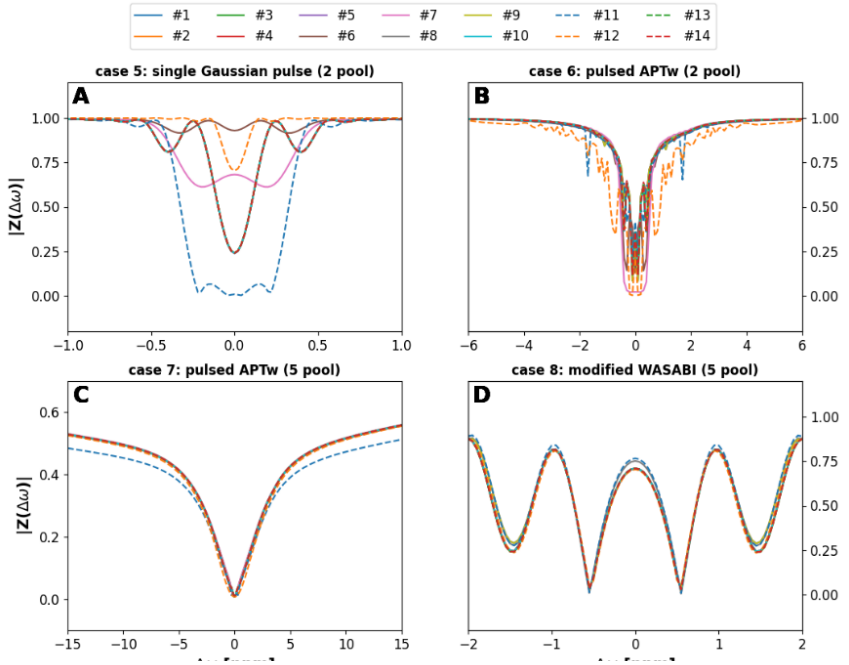

*Figure 1: Results for the 4 new cases for all 14 frameworks. (**A**) one single Gaussian-shaped RF pulse in a 2-pool model. (**B,C**) pulsed APTw preparation in a 2 pool (**B**) and 5 pool (**C**) model and (**D**) modified WASABI[5] with 2 block pulses.*

DISCUSSION: The large deviations observed in case 5 are highly likely attributable to incorrect implementations of the Gaussian-shaped RF pulse, which also explains why all groups/ frameworks showing deviations in case 5 deviate in case 6. It seems that the implementation of matching shaped pulse trains in different simulation frameworks, despite appearing straightforward, is very challenging. From the first study we know that the large deviation from #11 in case 7 results from a MT-Pool implementation considering only its z-component. The other deviations in this case are mitigated by the large influence of the MT pool, which leads to a reduced sensitivity towards variations in the shape and amplitude of the RF pulse.

CONCLUSION: Currently, quantitative CEST values determined using different BMC frameworks might not be comparable without their validation against each other. However, this study represents a significant advancement toward standardizing and improving the comparability of quantitative CEST parameters in future research.

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