Validate your CEST simulation!

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Declaration of
Financial Interests or Relationships

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I have no financial interests or relationships to disclose with regard to the subject matter of this presentation.

Motivation

- qCEST approaches (e.g., BMC fitting[1,2], CEST-MRF[3]) provide access to quantitative parameters like exchange rates or solute concentrations

- all methods rely on Bloch-McConnell equations

- reported qCEST values show strong deviations[4]

Do our BMC simulations differ?

Let's compare & validate them!
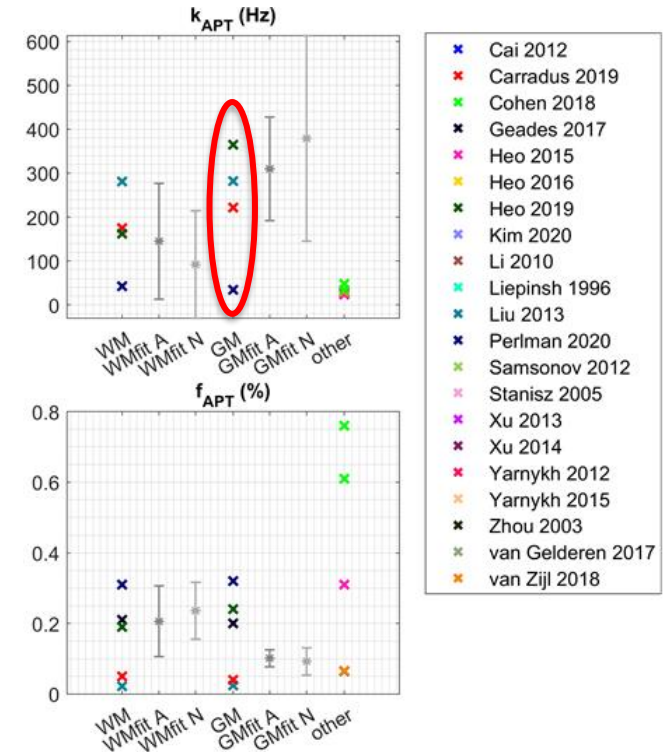
1. Zaiss *et al. NMR Biomed.* **32**, e4113 (2019)
2. Woessner *et al. Magn. Reson. Med.* **53**, 790–9 (2005)
3. Perlman *et al. NMR Biomed.* **e4710** (2022)
4. Zaiss *et al.* doi:10.1016/B978-0-12-822479-3.00040-3 (2021)

different preparations:

- steady-state APT CEST
- transient-state APT CEST
- WASABI

two different pool models:

- simple: creatine in water
- complex: WM-like tissue

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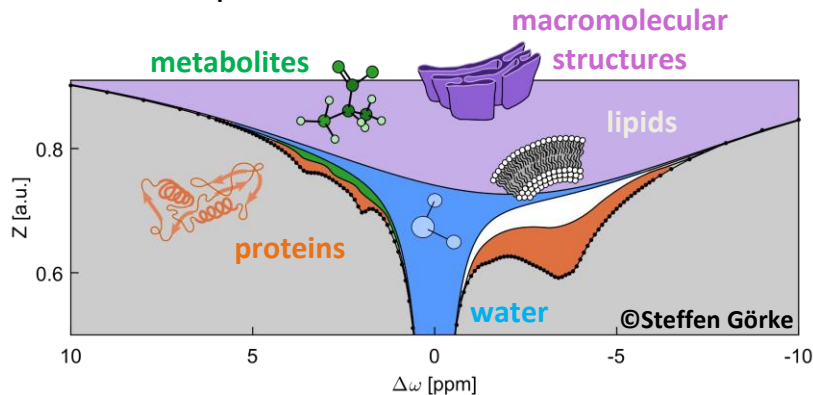
4 well-defined simulation cases:

"Reference" Z-spectra and MTR_{asym} curves

Simulation Study Details
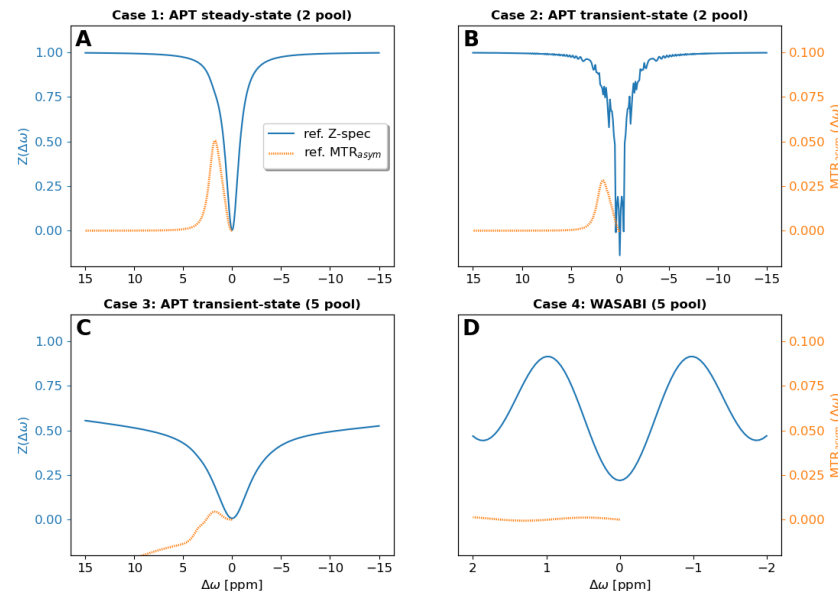
preparation schemes

Pulseq[1,2]

pool models

YAML
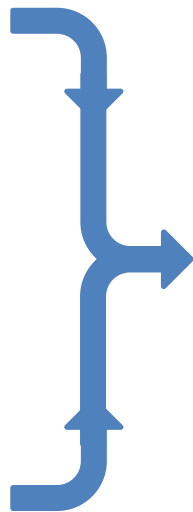
https://github.com/pulseq-cest/BMsim_challenge

GitHub

- a fully relaxed initial magnetization ($Z_i = 1$) for every offset
- post-preparation delay of 6.5 ms (mimic gradient spoiler)
- gyromagnetic ratio of exactly 42.5764 MHz/T
- field strength of 3T ($\omega_0 = 127.7292$ MHz/T)

1. Layton *et al. Magn. Reson. Med.* **77**, 1544–52 (2017)   2.   Ravi *et al. J. Open Source Softw.* **4**, 1725 (2019)
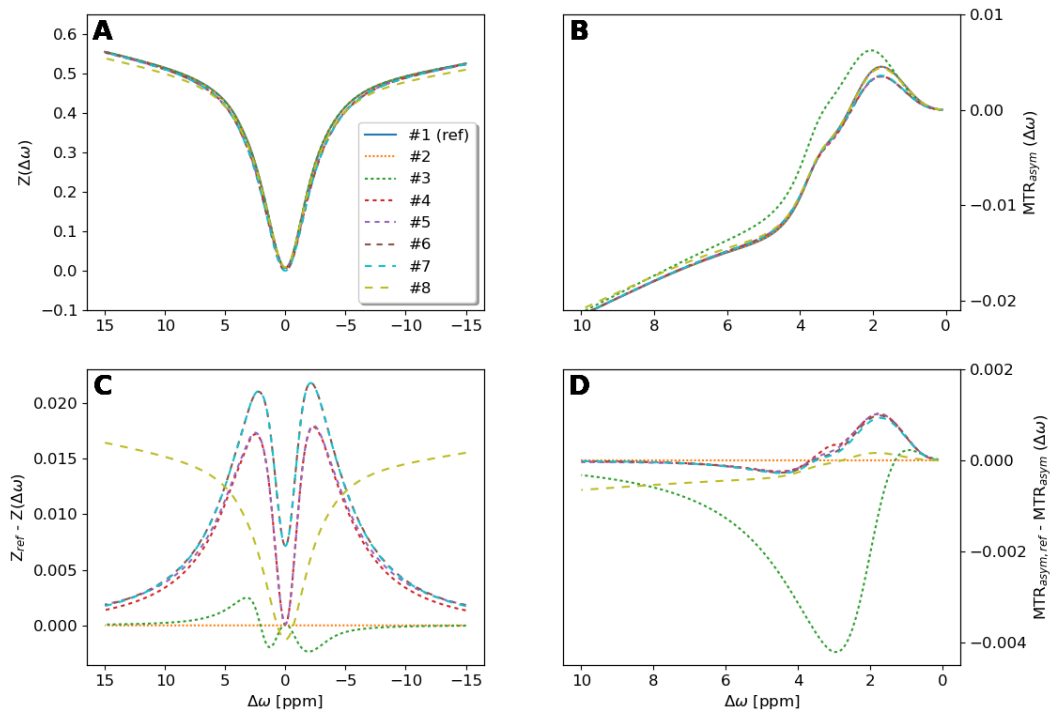
- pulseq-CEST[1] sim as reference (NOT the ground truth!)

- 5 different results for ΔZ-spec

- 4 different results for ΔMTR_{asym}

up to 100% deviation between MTR_{asym} values

1. Herz *et al. Magn. Reson. Med.* **86**, 1845–1858 (2021)

Current Results

- discussion with participants

- exchange with experts from MT community

➢ identify sources of deviations
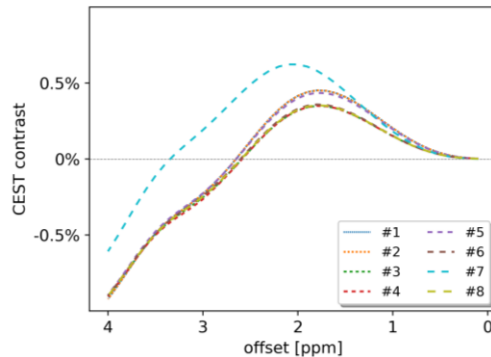
Nov. 2022   May 2023
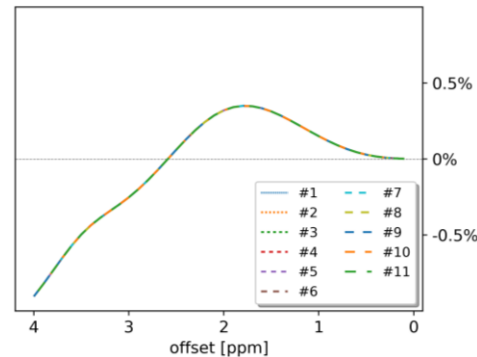
Summary of most important findings:
1. z-MT and xyz-MT are NOT interchangeable
2. simulation of post-preparation spoiler is mandatory

Online Evaluation Script

Outlook

publication of the study

- paper invitation by MRM
- currently preparing first draft

generalized Bloch model

match of z-MT and xyz-MT implementations?

2nd study with 4 additional cases

goal: include shaped pulse trains

➡️ **cover clinical CEST protocols**

case 5: 2 pool model, 272 shaped pulses (50 ms), 5 ms gaps
case 6: 2 pool model, 36 shaped pulses (50 ms), 5 ms gaps
case 7: 5 pool model, 36 shaped pulses (50 ms), 5 ms gaps
case 8: 5 pool model, 2 rect pulses (5 ms), 100 μs gap

Acknowledgements