



Validate your CEST simulation!

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Declaration of Financial Interests or Relationships

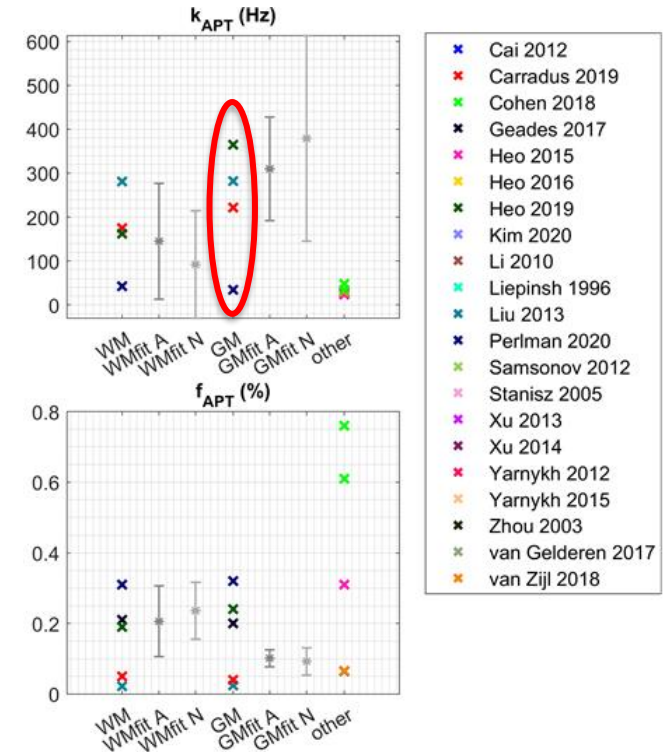
Speaker Name: Patrick Schuenke

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

- qCEST approaches (e.g., BMC fitting^{1,2}, CEST-MRF³) provide access to quantitative parameters like exchange rates or solute concentrations
- all methods rely on Bloch-McConnell equations
- reported qCEST values show strong deviations⁴

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)

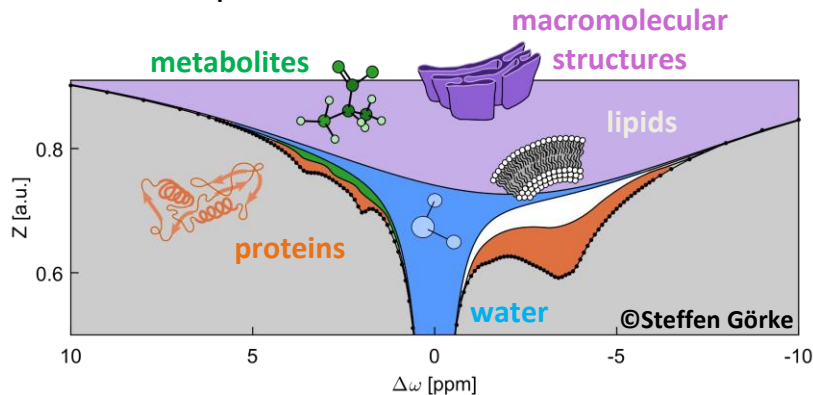
4. Zaiss et al. doi:10.1016/B978-0-12-822479-3.00040-3 (2021)

different preparations:

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

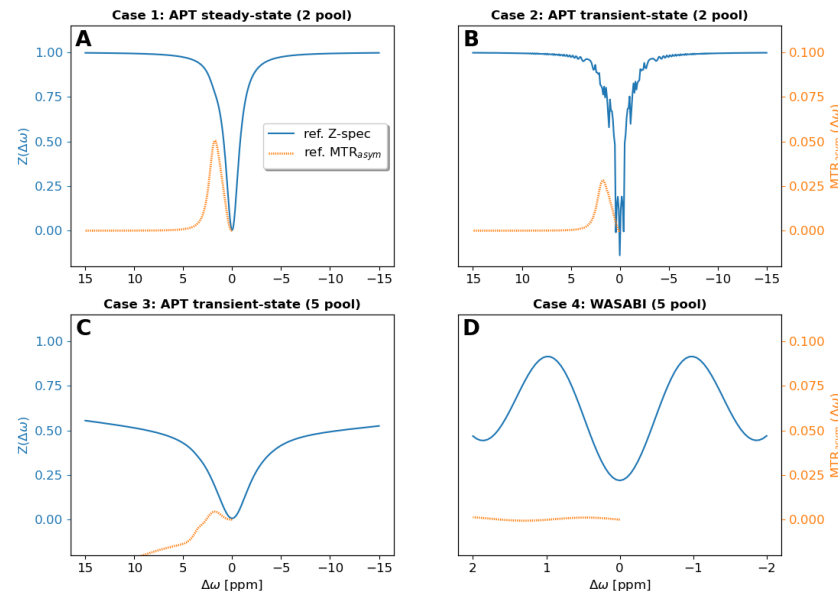
two different pool models:

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



4 well-defined simulation cases:

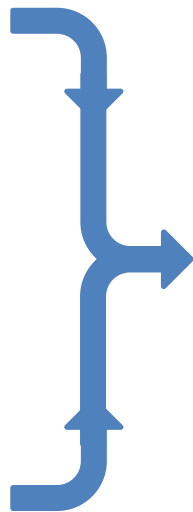
"Reference" Z-spectra and MTR_{asym} curves



preparation schemes



pool models

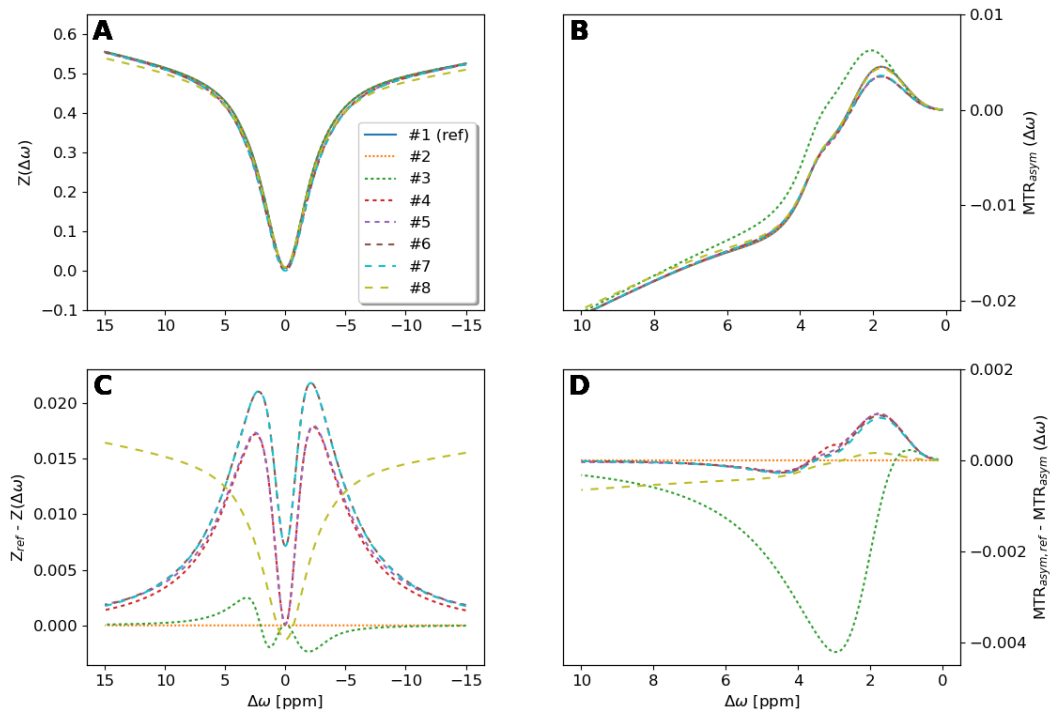


https://github.com/pulseseq-cest/BMsim_challenge



- 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)

Initial Results: Case 3 (2 μ T, 2s, 5 pool)



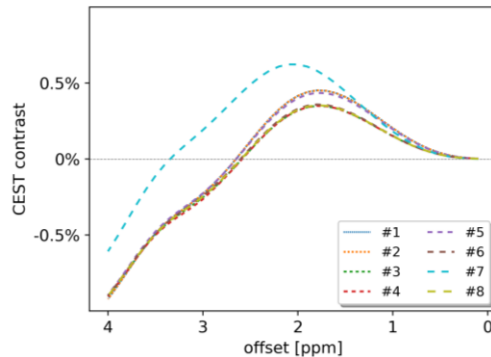
- pulseq-CEST¹ sim as reference (NOT the ground truth!)
- 5 different results for ΔZ -spec
- 4 different results for ΔMTR_{asym}

**up to 100% deviation
between MTR_{asym} values**

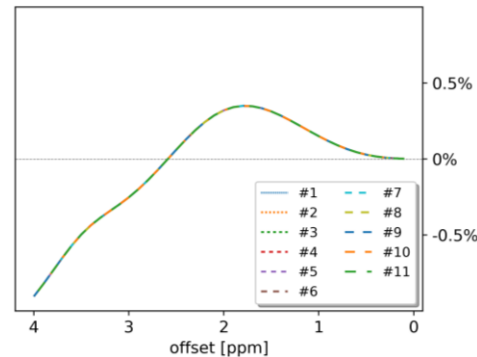
1. Herz et al. *Magn. Reson. Med.* **86**, 1845–1858 (2021)

- 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

PTB Online Evaluation Script



ValidateCESTSIM.ipynb ☆





Datei Bearbeiten Anzeige Einfügen Laufzeit Tools Hilfe Alle Änderungen wurden gespeichert

+ Code + Text

This Notebook evaluates the BMSim challenge data:

- https://docs.google.com/spreadsheets/d/1JN7VN-f1ktDrJgokb0FIUFwkH0MWYIPA_JSfnQoFOV
- described here https://github.com/pulseseq-cest/BMSim_challenge
- ISMRM abstract [here](#)

the first four cases are displayed in the image below.

Until now there are 4 sheets with different simulations		
case 1		2 pool Cr system -steady-state
case 2		2 pool Cr system
case 3		5 pool WM system
case 4		5 pool WM system



Please define case and settings here. CTRL+F9 to then run all.

Please select the case you want to compare:

case: 3

Exclude results for simulations considering only the z-component of the MT:

EXCLUDE_ZMT_SIMS: ☒

You can directly add own simulation data for the selected case here:

ADD_SIM_DATA: ☐

sim_data: 0.999542756 0.525369771 0.524773575 0.524176664 0.523579910 0.522982777 0.522384723 0.521786615 0.521187895

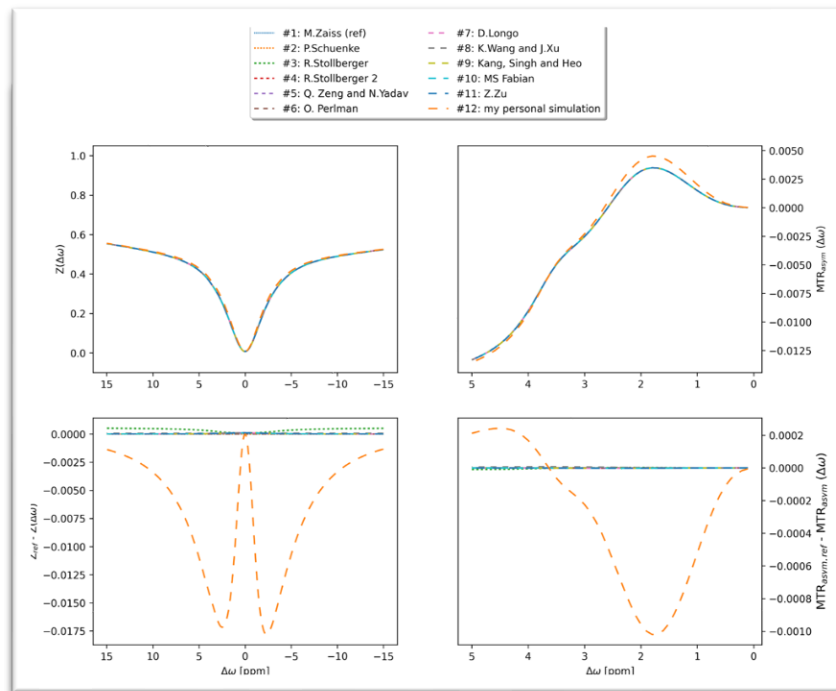
sim_data_label: my personal simulation

Or just add your results to the googlesheet linkend above.

Define the cutoff offset for the asymmetry plot:

ASYM_CUTOFF: 5

Code anzeigen



publication of the study

- paper invitation by MRM
- currently preparing first draft

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generalized Bloch model

RESEARCH ARTICLE | [Full Access](#)

Generalized Bloch model: A theory for pulsed magnetization transfer

Jakob Assländer ✉ Cem Gultekin, Sebastian Flassbeck, Steffen J. Glaser, Daniel K. Sodickson

First published: 23 November 2021 | <https://doi.org/10.1002/mrm.29071> | Citations: 1

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 μ s gap

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MAX-PLANCK-INSTITUT
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