Magnetic Resonance Imaging 34 (2016) 771–778

Contents lists available at ScienceDirect

Magnetic Resonance Imaging

journal homepage: www.mrijournal.com

Original contribution

Improvement of water saturation shift referencing by sequence and analysis optimization to enhance chemical exchange saturation transfer imaging

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ARTICLE INFO

Article history:
Received 17 December 2015
Revised 18 February 2016
Accepted 3 March 2016

Keywords:
Chemical exchange saturation transfer
Water saturation shift referencing
Monte-Carlo-simulations
Field inhomogeneity correction
Brain
Intervertebral disks

ABSTRACT

Purpose: To optimize B_0-field inhomogeneity correction for chemical exchange saturation transfer (CEST) imaging by investigating different water saturation shift referencing (WASSR) Z-spectrum shapes and different frequency correction techniques.
Methods: WASSR Z-spectra were simulated for different B_1-fields and pulse durations (PD). Two parameter settings were used for further simulations and experiments (WASSR1: $B_1 = 0.1\,\mu T$, PD = 50 ms; WASSR2: $B_1 = 0.3\,\mu T$, PD = 40 ms). Four frequency correction techniques were investigated: 1) MinW: Minimum of the spline-interpolated WASSR-spectrum; 2) MSCF: maximum symmetry center frequency algorithm; 3) PMSCF: further development of MSCF algorithm; 4) BFit: fit with Bloch equations. Performance of frequency correction was assessed with Monte-Carlo simulations and in-vivo MR examinations in the brain and intervertebral disks.
Results: Different shapes of WASSR-Z-spectra were obtained by changing B_1 and PD including spectra with one (1-Peak) or two (2-Peak) minima. WASSR1 resulted in 1-Peak WASSR-spectrum, whereas WASSR2 resulted in 2-Peak WASSR-spectrum. Both Monte-Carlo simulations and in-vivo MR examinations revealed highest accuracy of field-inhomogeneity correction with WASSR1 combined with PMSCF or BFit.
Conclusion: Using a WASSR sequence, which results in a Z-spectrum with a single absorption peak, in combination with advanced postprocessing algorithms enables improved B_0-field inhomogeneity correction for CEST imaging.

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1. Introduction

Biochemical imaging using chemical exchange saturation transfer (CEST) contrast is highly sensitive to magnetic field inhomogeneities [1,2]. These field inhomogeneities can shift the center of the Z-spectrum [2] and cause false results of CEST analysis.

Different methods to correct field inhomogeneities have been introduced. These methods include field maps, field inhomogeneity corrections using the minimum of either the Z-spectrum itself or of a fitted Z-spectrum (e.g. Lorentzian-shape fit, cubic spline fit or polynomial fit), and the maximum symmetry center frequency algorithm applied to a separately acquired water saturation shift referencing (WASSR) sequence [1,3–10]. WASSR has demonstrated the ability to be easily incorporated into CEST protocols along with robust performance across a variety of CEST applications [1,11–14].

A well-known phenomenon of CEST Z-spectra is that they can have different shapes including single or multiple minima due to different amount of direct water saturation (DWS) in dependence on pulse irradiation properties and different relaxation times [15–17]. The CEST effect depends on the field strength of the main magnetic field. Although the CEST effect is higher at high B_0 fields (7 T or higher), CEST measurements at lower field strengths have successfully detected exchangeable protons such as amide protons, amine protons and hydroxyl protons [12,18,19]. If human subjects are involved, measurements are usually realized at clinical MR systems. These clinical MR systems often have specific absorption rate (SAR) and hardware limitations and therefore pulsed CEST is used [17,20]. For WASSR data acquisition, it is not necessary to apply a pulsed acquisition scheme, since small B_1-fields and short durations of the radiofrequency irradiation keep SAR and hardware requirements in a feasible range. However, CEST imaging at clinical MR systems

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http://dx.doi.org/10.1016/j.mri.2016.03.013
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requires higher B_1-fields and therefore pulsed CEST acquisition has to be considered.

In this study, we aim to optimize the WASSR sequence and analysis software for an improved B_0 inhomogeneity correction on a clinical 3 T MRI system.

2. Materials and methods

Simulations and data analysis were performed using MATLAB (MathWorks, Natick, MA, R2012b).

2.1. Field inhomogeneity correction techniques

Four different field correction techniques were applied to the WASSR [1] data in our study:

i. The frequency offset was determined according to the minimum of the spline-interpolated WASSR data (*MinW*).
ii. The frequency offset was calculated with the *MSCF*-algorithm introduced by Kim et al. [1] (*MSCF*)
iii. A self-developed, enhanced version of the MSCF-algorithm was used: periodic MSCF-algorithm (*PMSCF*). Compared with the regular MSCF algorithm introduced by Kim et al. [1] the PMSCF algorithm includes all WASSR data to calculate the offset frequency. We aim to improve the accuracy of the algorithm by this method. Using the primary introduced WASSR algorithm, problems will occur including data at the boundaries. To avoid this problems, we extended the data according to
$Z(\omega_i + P) = Z(\omega_i) \mid P = \omega_{i=N} + \omega_{i=1} + \delta\omega;\ \delta\omega = \omega_{i+1} - \omega_i$ for all i
Thereby, $Z(\omega)$ is the normalized signal intensity at the offset frequency ω.
iv. The frequency offset was determined using a Bloch-fit (*BFit*). We fit the determined WASSR data using the method “nonlinear bisquare”. As fit model we used solution of the Bloch equations for our pulse sequence. We used the solution algorithm of Bloch equations as introduced by Murase et al. [21].

2.2. Numerical simulations

For all numerical simulations a magnetic field strength of 3 T was assumed. WASSR-spectra were calculated by solving the time course of spin magnetization using the Bloch equations [21,22]. Relaxation parameters for simulations were chosen representative of gray matter as $T_1 = 1331$ ms and $T_2 = 110$ ms [23].

WASSR-curves were simulated with $B_1 = 0.1$ μT and $B_1 = 0.3$ μT with varying pulse durations (PD) in the range of 0 ms to 50 ms with a step size of 1 ms. We used one Gaussian-shaped pulse for the simulation. The shape of the WASSR-curves were analyzed regarding the number of minima.

Two WASSR-curves with different shapes were used for further simulations: a) PD = 50 ms, $B_1 = 0.1$ μT (WASSR1); b) PD = 40 ms, $B_1 = 0.3$ μT (WASSR2). Z-spectra for these WASSR simulations were simulated in a range of −1.0 ppm to 1.0 ppm with a step size of 0.05 ppm.

To verify the accuracy of the above mentioned field inhomogeneity correction algorithms, $n_{simWASSR} = 10{,}000$ noisy frequency shifted WASSR-spectra were created by Monte-Carlo simulations. WASSR spectra with normally distributed offset ($\sigma_O = 0.1$ ppm) were calculated. Rician noise according to ref.[24, 25] was added with $\sigma_N = 0.025$, $\sigma_N = 0.05$ and $\sigma_N = 0.1$.

2.3. Accuracy of frequency correction

The frequency shift of each Monte-Carlo-simulated WASSR-spectrum was determined by the four techniques MinW, MSCF, PMSCF and BFit for WASSR1 and WASSR2. The residual error Δ (difference between calculated and original simulated frequency shift) was determined. Descriptive analysis of the residual error Δ was performed for both presaturation modules and for each frequency correction algorithm, respectively. Statistical analysis was performed using the Wilcoxon signed rank test. P-values below 0.05 were considered to be significant.

2.4. MR measurements

Two volunteers underwent MRI to show the transferability of our theoretically obtained results to in vivo measurements. The study was approved by the local ethics committee, and written informed consent was obtained from both volunteers. The examinations were performed on a clinical whole-body 3 T MR system (Magnetom Trio, A Tim System, Siemens Healthcare, Erlangen, Germany).

The first volunteer underwent an MRI examination of the brain. Signal reception was performed with a 12-channel birdcage head coil. The MR protocol (protocol 1) included a localizer, a CEST sequence for APT-CEST imaging, two WASSR data acquisitions with different B_1-amplitudes of the Gaussian-shaped presaturation pulse and, to differentiate white matter (WM) and gray matter (GM), a quantitative T_2-sequence. Single-slice turbo gradient echo imaging was used as host sequence for CEST and WASSR data acquisitions. Details of theses sequences are listed in Table 1. Parameters of the quantitative T_2 sequence were: FOV = 230 × 230 mm², basic resolution = 192 × 192, slice thickness = 6 mm, TE = [9.1, 18.2, 27.3, 36.4, 45.5, 54.6, 63.7, 72.8, 81.9, 91.0] ms, TR = 800 ms, flip angle = 180°, number of signal averages = 2, GRAPPA acceleration factor = 2.

The second volunteer underwent an MRI examination of lumbar intervertebral disks. Signal reception was performed with a spine matrix coil. The MR protocol (protocol 2) included a localizer, gagCEST imaging and two WASSR data acquisitions with different B_1-amplitudes of the presaturation module (Table 1).

In both examinations (brain and intervertebral disks), no shimming was performed between the CEST and both WASSR sequences, thus leading to the same center frequency of CEST and WASSR sequences.

For each acquired WASSR data, the four previously introduced algorithms (MinW, MSCF, PMSCF and BFit) were applied to obtain an offset map. These offset maps were further used to correct the acquired CEST spectra. MTR_{asym} maps were determined based on the corrected CEST spectra. Thereby, MTR_{asym} was evaluated in a range of 3.25 ppm to 3.75 ppm for APT-CEST imaging corresponding to the resonance frequency range of amide protons (resonance frequency at 3.5 ppm [26,27]) and in a range of 0.9 ppm to 1.1 ppm for gagCEST imaging corresponding to the resonance frequency range of hydroxyl protons (resonance frequency at 1 ppm [7]). MTR_{asym} was calculated according to

$$MTR_{asym}\left(\omega_{pool}, \Delta\omega\right) = mean\left(MTR_{asym}(\omega_i)\right)_{\omega_i \in \left[\omega_{pool} - \frac{\Delta\omega}{2},\ \omega_{pool} + \frac{\Delta\omega}{2}\right]}$$

where ω_{pool} is the pool position (1 ppm for gagCEST imaging and 3.5 ppm for APT-CEST imaging) and $\Delta\omega$ is the frequency range (0.2 ppm for gagCEST imaging and 0.5 ppm for APT-CEST imaging). We used a sample step size of $h = \omega_{i+1} - \omega_i = 0.01$ ppm.

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