The effect of the chemical shift displacement artefact on J-modulation in the STEAM sequence

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Introduction: The effects of the chemical shift displacement artefact (CSDA) on J-modulation of weakly coupled spins (AX_n), using the STEAM sequence, were demonstrated in previous studies [1, 2]. However, none of them have considered the effect of voxel displacement resultant from the first 90° pulse. Whereas in the PRESS sequence, the effect of this pulse can be neglected, due to the larger bandwidth of 90° pulses relative to 180° pulses [3], significant changes in the coupled-spin response in the STEAM sequence arise when a volumetric analysis is performed. The aim of this study is to derive an appropriate analytical model and compare the signal modulation obtained theoretically and experimentally.

Methods: *Analytical model.* A three dimensional compartment model was used to describe the combination of different RF patterns (3x3x3 = 27 compartments) undergone by the coupled spins in a conventional STEAM sequence. The configuration occurring in the plane where both A and X spins experience the first pulse is depicted in Figure 1 (compartments 19 to 27). The first 9 compartments represent the plane in which only X spins experience the first pulse and in compartments 10 to 18, only A spins experience the pulse. The product operator formalism was used to derive the expressions for the signal of the X spins resonance for each case, as described in [4]. The observable signal yielded by each spin in each compartment, as represented in Figure 1, resulted from a combination of coherence terms, where:

$$S_{A1} = \frac{1}{4} sin^2\left(\frac{\pi JTE}{2}\right)\cos^{n-1}\left(\frac{\pi JTE}{2}\right)\cos^{n-1}(\pi JTM)\cos(\Delta\Omega TM)\cos\left(\frac{\Delta\Omega TE}{2}\right);$$

$$S_{A2} = \frac{1}{4} sin^2\left(\frac{\pi JTE}{2}\right)\cos^{n-1}\left(\frac{\pi JTE}{2}\right)\cos^{n-1}(\pi JTM)\sin(\Delta\Omega TM)\sin\left(\frac{\Delta\Omega TE}{2}\right);$$

$$S_{A3} = \frac{1}{2} sin^2\left(\frac{\pi JTE}{2}\right)\cos^{n-1}\left(\frac{\pi JTE}{2}\right)\cos\left(\frac{\Delta\Omega TE}{2}\right);$$

$$S_{X1} = \frac{1}{2}\cos^2\left(\frac{\pi JTE}{2}\right);$$

$$S_{X2} = \frac{1}{4} sin^2\left(\frac{\pi JTE}{2}\right)\cos^{n-1}(\pi JTM)\cos(\Delta\Omega TM);$$

with $\Delta\Omega$ being the frequency difference (in $rads^{-1}$) between A and X spins.

2nd pulse: X 3rd pulse: A A: $2S_{A1}$ X: 0 20	2nd pulse: X 3rd pulse: A, X A: S_{A1} - S_{A2} X: S_{X1} 21	2nd pulse: X 3rd pulse: X A: 0 X: 1/2 19
2nd pulse: A, X 3rd pulse: A A: S_{A1} - S_{A2} X: - S_{X2} 26	2nd pulse: A, X 3rd pulse: A, X A: S_{A1} X: S_{X1} - S_{X2} 27	2nd pulse: A, X 3rd pulse: X A: 0 X: S_{X1} 25
2nd pulse: A 3rd pulse: A A: 0 X: 0 23	2nd pulse: A 3rd pulse: A, X A: 0 X: - S_{X2} 24	2nd pulse: A 3rd pulse: X A: S_{A3} X: 0 22

Figure 1 - Two dimensional compartment model related to the plane where both A and X spins experience the first pulse of the STEAM sequence. The signal contribution of each spin is shown in every compartment, identified by a number (19 to 27).

The signal from the remaining two planes is equivalent to the referred plane, but excludes the contributions related to the spin that does not feel the first pulse. The overall signal intensity in the VOI was calculated by performing a weighted sum of the signal and partial volumes of each compartment, as previously reported in [1], including a third dimension. *In vitro experiments.* Experimental data were also acquired to verify the simulations based on the derived analytical model, using a spherical 100 mM lactate phantom (AX_3 system) at two magnetic field strengths, 3 and 7T. All scans were performed on Philips Achieva MR systems (Philips Healthcare, Best, Netherlands). A series of 1H MR spectra were collected using the STEAM sequence (TE/TR = 144/2000 ms, 16 averages, 16 phase cycles, voxel volume = 40x40x40 mm3) with TM varied from 21 to 24 ms with a step size of 0.2 ms at 3T and from 17 to 18.3 ms with a step size of 0.1 ms at 7T. Water suppression was accomplished with an excitation method (BW = 140 Hz). Unsuppressed water spectra were also acquired before each scan. Area integration was used to quantify the lactate doublet (X spins), after normalization to the water signal.

Results: Figure 2 shows the contributions to the doublet signal from each of the 27 compartments, with the simulation parameters matching the experimental ones at 7T. Compartments in the plane where only X spins experience the first pulse (compartments 1 to 9) and the plane where both A and X spins experience the same pulse (compartments 19 to 27) were the ones that contributed the most to the overall signal. These compartments are marked in red in Figure 1 and are equivalent to the plane of cases 1 to 9. The simulated curves exhibit a close fit to the experimental data at both 3 and 7T, in terms of amplitude and frequency of modulation. A small shift in the phase of the curves (TM axis) is observable at both fields, which might indicate some lack of precision of the TM intervals defined by the MR scanner software. The 'ideal curves' were generated considering the case where the effects of the CSDA are not taken into account, i.e., all spins in the VOI experience all pulses, as derived in [4].

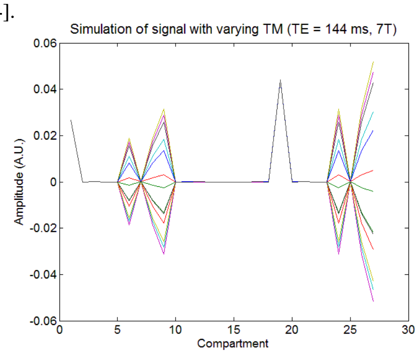

Figure 2 - Simulation of the lactate doublet signal in each of the 27 compartments, with varying TM. The parameters used were the same as for the experimental 7T data.

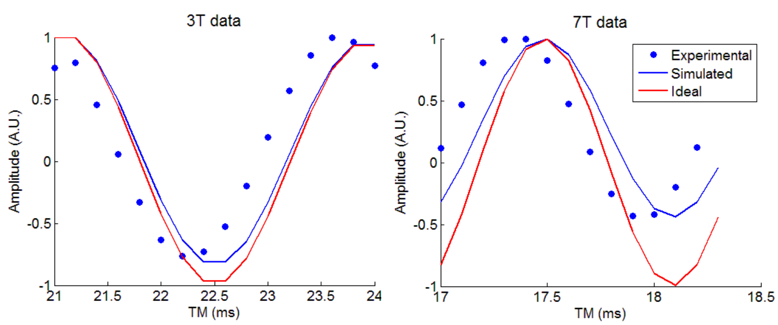

Figure 3 - Experimental and simulated data at 3 and 7T for lactate. The 'ideal curves' represent the signal from the compartment where both A and X spins undergo all the pulses. The BWs of the 90° pulses considered were 1987 and 2207 Hz, for 3 and 7T, respectively.

Discussion: This work demonstrates the importance of considering the effects of all pulses on the modulation pattern of weakly coupled spins, especially at ultra-high magnetic field strengths. This model provides a means to predict the resulting lineshapes of metabolites of AX_n form, constituting a tool for optimization of sequence timing parameters.

References: [1] Wooten et al., Proc. Intl. Soc. Mag. Reson. Med., 9 (2001); [2] Thompson and Allen, Magn. Reson. Med., 45: 955-965 (2001); [3] Edden et al., Magn. Reson. Med., 56: 912-917 (2006); [4] Wilman and Allen, J. Magn. Reson., 101: 102-105 (1993).

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