LINESHAPE COMPENSATION METHODS FOR MODELING OF 2DJ SPECTRA

Victor Javier Adalid[1], Chris Boesch[1], Christine S. Bolliger[1], and Roland Kreis[1]
[1]Depts. Radiology and Clinical Research, University Bern, Bern, Switzerland

Purpose: To account for imperfect lineshapes when model-fitting 2D MR spectra

Introduction: Inhomogeneities in magnetic field and eddy currents cause the lineshape (LS) for metabolites and water to deviate from the ideal Lorentzian type. Various approaches have been used to correct this distortion for 1D spectra [1-4] based on water as reference line or B_0 field maps or to define the LS in fitting. However, for in vivo 2D spectra, this has not been widely studied [5,6]. Restoring the original LS by deconvolution methods usually modifies the noise profile and/or introduces spikes. Here, a method is tested where the reference LS is applied to the model in order to fit the distorted spectra with equally distorted basis spectra, in particular as applied to 2DJ data with maximum echo sampling ((MES): data sampling started right after the 2nd 180 pulse).

Methods: To test the methods, simulated 2DJ brain spectra were created (4 kHz width, 8 TE: TE=20, 40, .. 160 ms). MES PRESS model spectra were generated in VESPA [7] at 3T for six metabolites: creatine, glutamate, glutamine, glycerophosphorylcholine, myo-inositol, NAA. Metabolite T_2's typical for brain were used. Macromolecule spectra were added for the first 4 TE. They had been obtained experimentally earlier (average from 10 subjects, gray matter, 3T, metabolite-nulled with inversion time of 900 ms). A dataset for the unsuppressed water signal was also created assuming a T_2 of 60 ms. Several LSs have been evaluated. This report deals with a LS distortion defined as asymmetric triangles in frequency domain (2 Hz up, 15, 25, or 50 Hz down ($\rightarrow$ half height widths (LW) of 7.5, 12.1, and 25.4 Hz)), applied in time domain (TD) upon each echo, centered at echo maximum. Three SNR levels (62, 43, 28, defined for NAA in the undistorted case) with 10 noise realizations each were evaluated.
To obtain the LS, the water TD signal was corrected for its T_2-related exponential decay, where this T_2 had been obtained from the TE signal decay.
Three different methods of LS correction are compared to fitting the distorted signals directly. (A) *Eddy Current Correction (ECC)* [1]: Complex division in TD by the phase of the LS. (B) *QUALITY [2] deconvolution*: complex division by the LS in TD. (C) *QUECC* [3]: QUECC combines QUALITY for the first part of the FID with ECC for the rest; here adapted for the 2D MSE case by applying QUALITY for the inner data range around the echo maximum and ECC outside, with the transition points based on SNR thresholds for both the water and the metabolite data (continuity of amplitude scaling enforced). (D) *Lineshape-enhanced-model (LEM)*: The LS is applied to the model of the metabolites in TD that are then used as model to fit the distorted data. In addition, "ground truth" fit results were obtained by fitting spectra without distortion, and uncorrected distorted spectra were fit for comparison.
Simultaneous fitting of the 2D data sets was performed in FiTAID [8] using a bounded Levenberg-Marquardt algorithm in frequency domain.

Results: Sample data and fits for one case of the tested 2DJ spectra distorted by a triangular LS is presented in the Figure. Four ways to compensate for the distortion are illustrated in comparison to the undistorted case and the non-compensated data and fit. ECC, QUALITY and QUECC restore a narrow LS, but are plagued with higher noise, while LEM provides an adapted model to fit the distorted spectra. The performance of these methods
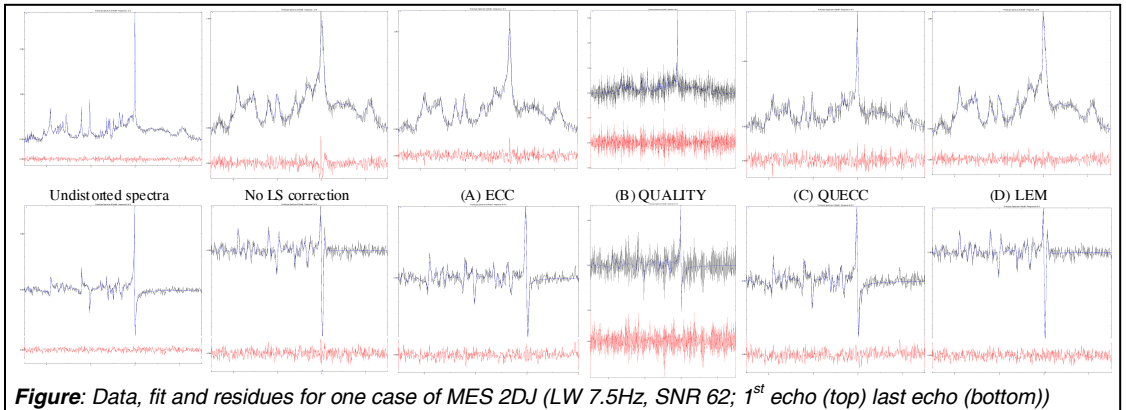

Figure: Data, fit and residues for one case of MES 2DJ (LW 7.5Hz, SNR 62; 1st echo (top) last echo (bottom))

is summarized in the Table. For brevity, only average data for the area parameters of metabolites with a large singlet (creatine, GCP, NAA) is given. With the current implementations, it appears that both QUALITY and QUECC show considerable bias, while ECC (for small LW) and in particular LEM result in smallest bias and variance. The same trend is seen also for the other metabolites, but they mostly show larger bias and variance (in particular glutamine).

Discussion and Conclusions: Given the presented results and further evaluations, it appears that LEM, i.e. including the distortion in the model, may be a better approach than trying to deconvolve the spectra with the estimated LS and then fit the model with ideal LS, especially so, for large distortions. However, the situation is very complex and the results are bound to depend on the exact nature of the distortion, the SNR of metabolites and water, but also the tunable parameters in QUECC (or Wiener filtering, which is also evaluated). In addition, one should keep in mind that in the current evaluation the distortion is perfectly imprinted in the water signal, while in vivo a) the chemical shift artifact may cause a ppm-dependence of the exact shape of the distortion, and b) the water signal can be due to multiple compartments with differing T_2s making the extraction of the LS more cumbersome.

LW	Bias [%] for areas						Variance [%] for areas					
	Undist.	*No corr.*	*ECC*	*QUA-LITY*	*QUECC*	*LEM*	*Undist.*	*No corr.*	*ECC*	*QUA-LITY*	*QUECC*	*LEM*
7.5 Hz	0.7%	1.3%	1.0%	4.0%	11.1%	0.8%	2.3%	4.4%	4.3%	17.3%	7.1%	4.2%
12 Hz		2.7%	1.3%	4.0%	15.9%	1.9%		5.3%	5.3%	21.0%	11.2%	5.4%
25 Hz		8.3%	11.9%	8.7%	19.3%	1.4%		7.1%	14.3%	31.4%	12.0%	8.0%

Table: Bias and variance of estimated area values (mean area values for singlet resonances averaged over noise realizations and SNR levels)

References: [1] Klose MRM 14:26 (1990); [2] de Graaf et al. MRM 13:343 (1990); [3] Bartha et al. MRM 44:641 (2000); [4] An et al. MRM 72:903 (2014); [5] Kreis et al MRM 54:761 (2005); [6] Fuchs et al. MRM 71:458 (2014); [7] https://scion.duhs.duke.edu/vespa/; [8] Chong et al. MAGMA 24:147 (2011).