Lipid T2* Determination by Modeling the Intra-Molecular Chemical Shift Effect

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Introduction: The measurement of T2* and/or T2† (which is derived from T2* and T2) are important for the quantification of physiological events or pathologies related to susceptibility changes in tissue. In bone, for example, changes in T2† and T2* are caused by susceptibility changes between the trabecular bone and bone marrow and it has been shown that T2* and T2† correlate with the changes in bone microstructure [1-3].

Since bone marrow has both a water and a fat component, the signal decay versus time in T2* measurements depend on the properties and ratios of these two species. One phenomenon that is usually ignored in modeling the T2* signal decay of fat is the intra-molecular chemical shift. Different from water, which has two magnetically equivalent hydrogen atoms (and thus resonating at the same frequency), the hydrogen atoms that make up the fat molecule are not magnetically equivalent. Thus different groups within the fat molecule resonate at different frequencies [4]. The main lipid peak (formed mainly by the CH_2 groups in the molecule) resonates at ~1.2 ppm whereas the terminal CH_3 groups resonate at ~0.8 ppm. This chemical shift difference causes a modulation in the T2* decay curve and the single exponential approximation, typically used to fit T2*, leads to erroneous results.

In this work we present a signal equation model for extracting T2* for fat, minimizing the effects of the intra-molecular chemical shift.

Theory: If we approximate the CH_2 and CH_3 peaks with delta functions, the signal decay magnitude I for a pure lipid sample can be modeled by Eq. 1, where C_s is the relative chemical shift between the CH_2 and CH_3 resonances, and I_{CH2}, I_{CH3} are the magnitudes of each peak. This equation is a non-linear function of the unknown parameters, and thus must be fitted using a non-linear least squares technique. The Levenberg-Marquardt algorithm was used for this study.

$$I = \left\| I_{CH2} + I_{CH3}\exp(iC_sTE) \right\| \exp(-TE/T2^*) \qquad (1)$$

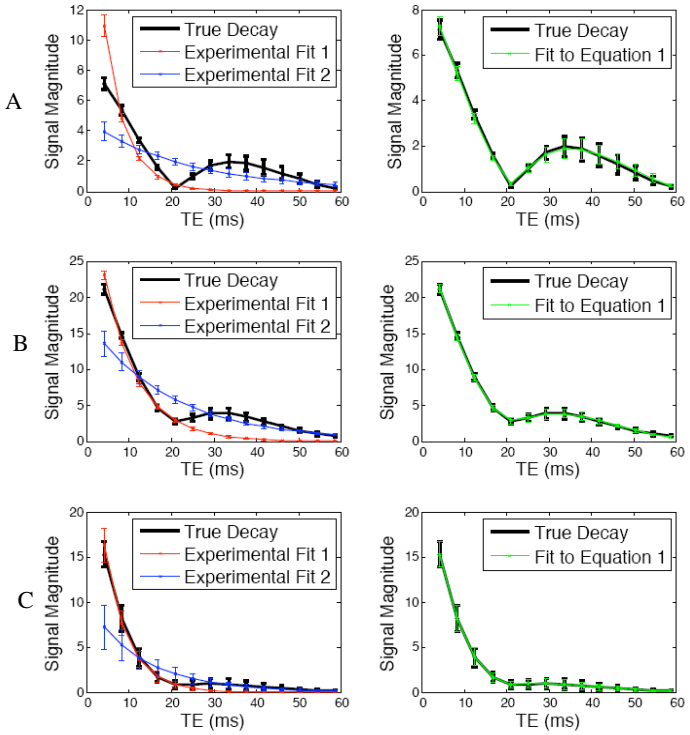

Figure 1

Methods: In order to test the model we measure T2* in compounds mimicking human fat (hexane and baby oil). Images were acquired at 1.5T on a GE Signa NV-CV/i scanner, with a spoiled gradient echo pulse sequence (flip angle=90, TR=500, NEX=1, BW=±32kHz) at 14 TE values ranging from 4.2 to 58.8 ms. For baby oil, we performed spectroscopic experiments at 11.7 T in order to determine the ratio of the CH_2/CH_3 peaks and their chemical shift differences. At this high field, the resonances corresponding to the CH_2 and CH_3 groups were resolved thus the ratio and chemical shifts for these two groups were easily estimated. For hexane, the CH_2/CH_3 ratio was determined from the molecular structure and their chemical shift differences from the literature.

Results: Figure 1 shows the signal decay versus TE curves for (A) hexane (B) baby oil, and (C) a phantom containing a sponge embedded in baby oil (the sponge is used to reduce T2*). The data in black are the measured points. The red and blue curves (shown in the left panel of Fig. 1) are the experimental fits to the data using the single exponential decay typically used for T2* measurements (ie, $I=I_o\exp(-TE/T2^*)$). In the fitting represented by the blue curves we only used data points in the 4.2 to 21 ms TE range. In the fitting represented by the blue curves we used the full range of TE values. The green curves (shown in the right panel of Fig. 1) represent the fitting of the data to Eq. 1. In general, the single exponential does not fit the data properly and the calculated T2* values (Table 1) depend on the range of points used. On the other hand, Eq. 1 fits the data well thus we can expect a more accurate calculation of the T2* value. Also note that the calculated CH_2/CH_3 ratio and the CH_2/CH_3 chemical shift differences match well the expected values.

Table 1

SAMPLES	T2* ESTIMATES (ms)			CH_3/CH_2 PEAK RATIO		CH_3/CH_2 CHEM SHIFT (ppm)	
	Fit to Eq. 1	Single Exponential Fit (TE range: 4.2-21 ms)	Single Exponential Fit (TE range: 4.2-58.8 ms)	Fit to Eq. 1	Expected value	Fit to Eq. 1	Expected value
Hexane	24.6±4.3	5.2±0.3	32.8±8.7	0.73±0.09	0.75	0.37±0.01	0.40
Oil	20.1±0.4	8.1±0.5	20.9±2.3	0.56±0.06	0.62	0.38±0.02	0.42
Oil + Sponge	9.9±2.3	5.6±0.7	12.3±2.7	0.61±0.10	0.62	0.36±0.03	0.42

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References: [1] Wehrli FH et al Radiology 2000; 217, 527. [2] Link TM et al Radiology 1998; 209. [3] Majumdar S, et al JMRI 1992; 2:209. [4] Wehrli FH et al Magn Reson Imaging, 5; 157, 1987.