Effects of T₂ relaxation and diffusion on longitudinal magnetization state and signal build for HOMOGENIZED cross peaks

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¹Optical Sciences Center, University of Arizona, Tucson, AZ, United States, ²Department of Radiology, Arizona Health Sciences Center, Tucson, AZ, United States **Motivation:** HOMOGENIZED¹ and the recently proposed IDEAL² sequences have great potential for in-vivo spectroscopy³. Diffusion weighting in HOMOGENIZED is present both to give intentional diffusion weighting and as a side effect of the various gradients. Stekjsal-Tanner (ST) diffusion weighting⁴ during the mixing (t₁) and echo (t₂) periods of the sequence can be used to suppress radiation dampening and provide enhanced diffusion weighting⁵. There is an additional diffusion weighting possible, due to the iZQC gradient (zq) and β pulse combination. This weighting does not behave as ST diffusion weighting. Kennedy et al.⁶ have shown recently that this diffusion weighting has the novel property of being insensitive to object motion. **Discussion:** We have concentrated our efforts on the 2d iZQC HOMOGENIZED sequence shown to the right: ZQ

The sequence consists of three RF pulses, α for excitation, β to convert helical transverse magnetization to spatially modulated M_z, and π to form a spin echo. The a₁ a₂ gradient pair yields ST diffusion weighting and radiation damping suppression during t₁. The b₁, b₂ gradient pair accomplishes the same for t₂. The c₁, c₂ gradient pairs crush transverse magnetization created at π due to pulse imperfections and B₁ inhomogeneity. The zq gradient selects



intermolecular zero quantum coherences (iZQCs) in the quantum picture. In the classical picture the zq gradient in combination with β creates spatially modulated z magnetization whose magnetic field causes unwinding (and eventually rewinding) of helically twisted transverse magnetization.

A 2d experiment is carried out by incrementing t_1 over multiple acquisitions. In a two (or multiple) component system where only one component is present in high concentration (the solvent S), cross peaks with the solute component of interest (I) will be formed at (F₁, F₂)=(I-S, I) the "p" type iZQC and (S-I, I) the "n" type iZQC. Axial iZQC peaks are formed at (0, I) and (0, S). The equation for peak magnitudes, neglecting radiation damping, T₂ relaxation, and diffusion has been described in the literature⁷.

Results: For the first time, to the authors' knowledge, an analytical expression for the cross peak magnitude in the presence of diffusion and T_2 relaxation has been developed. It is valid as long as S and I are separated by $1/\tau_s$ in frequency, so that only longitudinal S magnetization contributes to signal build. As long as the a and b gradient areas are chosen correctly, radiation dampening is not significant. Some preliminary definitions precede the expression, notation is as per Ahn et al.⁷

$$q_{zq} \equiv \frac{\gamma G_{zq} \delta_{zq}}{2\pi} \quad \tau_{Seff} \equiv \tau_{S} e^{(b_{a}+b_{zq})D_{S}} e^{\frac{t_{1}}{T_{2}^{S}}} \quad F(t_{z}) \equiv \frac{1-e^{-t_{2}\left(2\pi q_{zq}\right)^{2}D_{S}}}{\tau_{Seff}\left(2\pi q_{zq}\right)^{2}D_{S}} \quad M_{P} = -M_{0}e^{-(b_{a}+b_{zq}+b_{b})D_{I}} e^{-\frac{(t_{1}+t_{2})}{T_{2}^{I}}} \cos\left(\beta\right)J_{1}\left[-\sin\left(\beta\right)\frac{2}{3}F(t_{2})\right]$$

 q_{zq} is the spatial frequency of periodic z magnetization M_z formed by G_{zq} and β . τ_S is the dipolar demagnetization time for spin S and a τ_{Seff} has been defined to take account of T_2 and diffusion losses (ST b-values, b_a and b_{zq}) incurred during t_1 before beta transforms into M_z . $F(t_2)$ can be thought of as an exponentially slowing "winding" parameter, instead of the linear winding parameter t_2/τ_S when diffusion is negligible. M_p is the p type cross peak magnitude; a similar expression has been found for M_n as well.

The effect of $F(t_2)$ is to stretch the time axis when diffusion weighting is significant. Three theoretical situations are shown in Fig. 1. Comparison of the predicted cross peak magnitude with experiment is shown in Fig. 2. The solvent is water at room temperature, the solute TSP at 100mM concentration. Field strength is 4.7T yielding τ_s =200ms. Other effects such as B1 inhomogeneity and RF pulse error contribute to lengthen τ_{seff} (reduce available S magnetization). The expression should be useful for optimization of HOMOGENIZED experiments, and general understanding of iZQC signal behavior.

References:

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Fig. 1 – Plot of theoretical cross peak magnitude M_p vs. t_2 , negligible T_2 decay. Y axis is in units of M_0 . Three situations are shown: **Black** – negligible diffusion, the oscillatory behavior is evident. **Dark Gray** – diffusion of M_z has delayed the maximum and stretched the subsequent portion of the curve to longer times. Light Gray – M_z modulation has completely diffused away before the maximum can be obtained.

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Fig. 2 – Data points and theoretical curve for three cases. Y axis arbitrary units. Upper - TR=20s β =90° G=10mT/m Middle - TR=20s β =90° G=40mT

Lower - TR=2s β =90° G=40mT/m