Experimental Parameters and Diffraction Patterns at High q Diffusion MR: Experiments and Theoretical Simulations

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Introduction

q-Space diffusion MR [1, 2], is increasingly being used to obtain structural information in neuronal tissues [3-7] on a micron scale, well below the resolution in conventional MRI. Diffraction pattern in q-space diffusion MR obtained from packs of impermeable micro-capillaries exhibits a strong angular dependence [8]. Recently the 3-D restricted model of water diffusion embodied in the Composite Hindered and Restricted Model of Diffusion (CHARMED) framework, originally developed to describe water diffusion in white matter [9, 10] was shown to predict this peculiar angular dependence. Here we have characterized the peculiar signal decay in such micro-capillaries when the SGP approximation and more importantly the $\delta \ll \Delta$ condition are violated both experimentally and by the restricted model embodied in the CHARMED framework. We found good agreement between experimental results and the CHARMED model even under these conditions thus providing further confirmation of the CHARMED model.

Methods

NMR diffusion experiments were performed on packs of 4-cm hollow cylindrical tubes (micro-capillaries) having a diameter of 20µm (Polymicro Technologies), using an 8.4T NMR spectrometer equipped with a Micro5 gradient system capable of producing pulse gradients of up to 190 gauss/cm in each of the three directions. The micro-capillaries were filled with water and aligned along the z-axis in the magnet. A diffusion weighted stimulated echo sequence was used with the following parameters: TR = 3000 ms, TE= 80ms, δ= 32ms with diffusion gradient pulses incremented to the maximal value (G_{max}) of 10 gauss/cm in 32 steps. In these experiments Δ was set to 40, 100 or 300ms. In addition, experiments with TR/TE/δ =3000/112/48 were also collected with Δ of 60, 100, 200 and 400 ms. Here the diffusion gradient pulses were incremented to the maximal value (G_{max}) of 6.67 gauss/cm in 32 steps, thus resulting in q_{max} of 1362 cm^{-1} in both sets of experiments. Signal attenuation as a function of q-values was measured for different rotational angles (α) with respect to the +z from 0^0 to 180^0 (see Figure 1). Simulations were performed using the restricted component of the CHARMED model using an in-house Matlab program.

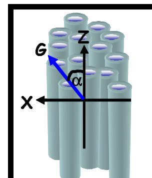

Figure 1

Results

Figures 2A-B shows the experimental and simulated signal decay as a function of the q-values in 20 µm tubes for different αs when δ was 32 ms and Δ was set to 42 and 100 ms, respectively. Clearly one observes good agreement between simulations and the experimental results. When the δ/Δ ratio was 3.1, as in Fig. 2B, there is a very good agreement between simulations and experimental results while when this value is nearly 1.3, diffraction appears in the same q-values in the simulations and experiments. However, there the experimental signal decay and the simulations are less similar. Surprisingly when the δ/Δ ratio was nearly 1.3 diffractions appear, both in experiments and simulations, at higher q-values. This implies that one would extract smaller values for the restricting compartment under these conditions. This is demonstrated nicely in Fig. 2C which shows experimental and simulated signal decay for $\alpha = 90^0$ when the diffusion time was set to 42, 100 and 300 ms. For Δ of 40ms diffraction appears at higher q-values both in the experiment and simulation. Figure 2D shows the same data along with the simulations obtained from the CHARMED model for experiments acquired with δ of 48 ms and Δ of 60, 100, 200 and 400 ms. This figure shows excellent agreement between experimental results and the predictions of the 3-D model of restricted diffusion within CHARMED framework for Δ equal or higher than 100ms.

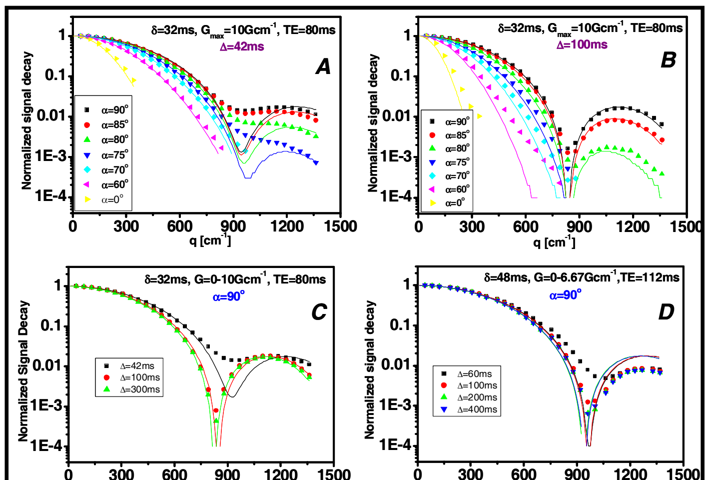

Figure 2

Discussion

Importantly, we found that the restricted part of the CHARMED model can describe accurately the signal decay and the peculiar dependency of the diffraction pattern on the rotation angle for wide range of experimental conditions including those violating the SGP approximation and the $\delta \ll \Delta$ conditions. It is important to note that here experiments were performed with experimental parameters (gradient strength) which approach those obtainable on clinical scanners. This behavior follows because the net signal attenuation can be written as the product of two terms, one describing the 1-D Gaussian diffusion along the free axis of the tubes, and another describing the restricted diffusion perpendicular to the axis of the tubes. The former dominates the latter at most angles except when displacements are probed perpendicular to the tube walls. This study provides further support to the validity of the assumptions embodied in the CHARMED model.

References

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