Comparing diffusion-weighted MRI signals from ordered and disordered microstructures

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Target audience: Those interested in microstructural modelling of the diffusion signal from spherical cell geometries, for use in tumour imaging.

Purpose: Various microstructural tissue models used for simulating/modelling diffusion-weighted (DW) MRI data are comprised of cells with idealised shapes in an ordered packing geometry, for example hexagonally packed cylinders[1] or spheres on a face-centred cubic lattice[2]. Recent work in 2D has shown that the time-dependent extra-cellular diffusion coefficient exhibits different trends in ordered and disordered environments[3], suggesting that the effects of disorder should be included when modelling DW-MRI data from tissue with disordered microstructure. Here we use Monte Carlo simulations in 3D to compare the DW-MRI signal obtained from diffusion experiments in ordered and disordered environments, using pulse sequence parameters available on clinical scanners.

Methods: Diffusion simulations (3D random walk with spatial and temporal resolutions of 0.655 μm and 0.0357 ms, respectively) were performed using a simple tissue model comprised of impermeable spherical cells with a radius of 9.48 μm. Diffusion in ordered and disordered systems was studied by running separate simulations for hexagonally packed cells and randomly packed cells; for both systems the intra-cellular volume fraction was 0.62. For both packing geometries, two separate experiments were performed: first, diffusion in the extra-cellular space alone was simulated; second, diffusion in both the intra- and extra-cellular spaces was simulated. All diffusion coefficients were 2 μm^2/ms. Pulsed gradient spin-echo (PGSE) signals were synthesised from each simulation using the following gradient strengths, G, separations, Δ, and duration, δ: G={0,5…80} mT/m, Δ={30,110} ms and δ=10 ms. All simulations were performed with Camino[4,5], and the disordered sphere packing was achieved using a modified Lubachevsky-Stillinger algorithm[6,7] (cherrypit.princeton.edu/Packing/C++/). The ordered and disordered geometries are shown in Fig. 1, along with the corresponding pair correlation function, g_2. The g_2 plot for the disordered packing (bottom) is qualitatively different from the series of delta function peaks characteristic of ordered packing (top).

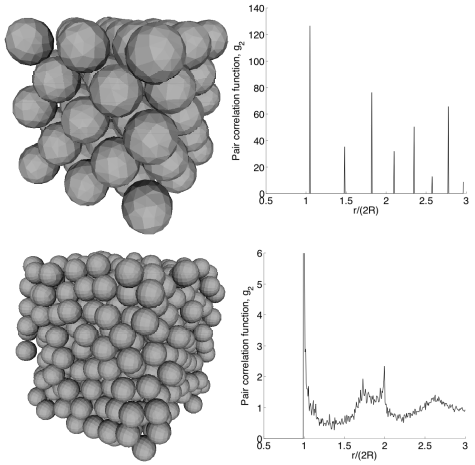

Fig. 1. Packing geometries (not to scale) and corresponding pair correlation functions, g_2, for ordered and disordered packing (top and bottom, respectively).

Results and discussion: Plots of the normalised synthesised PGSE signals, S, as a function of G and Δ are shown in Fig. 2, for the extra-cellular diffusion simulations (left) and for the combined intra- and extra-cellular diffusion simulations (right). In general there is little difference between signals from the ordered and disordered packing (crosses and circles in Fig. 2 plots, respectively). The greatest difference is observed for extra-cellular diffusion when using large gradient strengths (maximum S difference ≈ 0.01). However, as shown in the right hand panel of Fig. 2, these differences are even smaller when simulating the more realistic situation where diffusion takes place in both the intra- and extra-cellular spaces (maximum S difference ≈ 0.004). Here we see essentially no difference between ordered and disordered signals, over a range of clinically relevant pulse sequence parameters. These results suggest that the diffusion signal cannot distinguish between ordered and disordered diffusion environments, at least over the range of pulse sequence parameters and tissue properties investigated here.

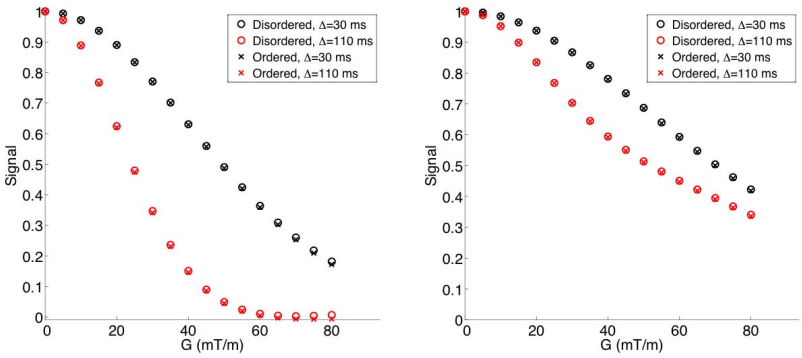

Fig. 2. Simulated signals as a function of G and Δ for ordered and disordered packing (crosses and circles, respectively) using extra-cellular diffusion (left) and combined intra- and extra-cellular diffusion (right).

Conclusion: Small differences in DW-MRI signals were observed between ordered and disordered environments when extra-cellular diffusion was studied with G>60 mT/m. However, signal differences were found to be negligible when combined intra- and extra-cellular diffusion was simulated. This suggests that the diffusion signal is insensitive to the packing geometry's order/disorder, for the sequence parameters and tissue properties covered here.

References: 1. Meier et al. MRM 2003;50:500–509. **2.** Xu et al. MRI 2011;29:380–390. **3.** Burcaw et al. ISMRM 2013:495. **4.** Cook et al. ISMRM 2006;14:2759. **5.** Hall and Alexander. IEEE Trans Med Imaging 2009;28:1354-1364. **6.** Skoge et al. Phys Rev E 2006;74:041127. **7.** Donev et al. J Comp Phys 2005;202:737–764.

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