Numerical Simulation of Double Wave Vector Diffusion Experiments

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INTRODUCTION

In many situations applications of diffusion weighted imaging suffer from ambiguous results. This is in part due to the large number of parameters that affect the diffusional motion of water in a restricting geometry such as living tissue. In recent times, experiments have gained new interest where two successive gradient pulse pairs of different direction are used between excitation and acquisition (double wave vector diffusion weighting, DWV) [1,2]. DWV weighting might provide a means to acquire more detailed information on the tissue structure, such as cell size and shape. P. P. Mitra [3] developed a theoretical description of double wave vector experiments which is valid under the assumption of infinitely short gradient pulses and long diffusion times, and which has not yet been verified experimentally. In the numerical simulations described here we test the theoretical description given by Mitra in a situation where the approximating assumptions are not strictly met. We show how the dependence of the signal on the angle between the diffusion gradient directions changes its shape upon variation of the waiting period between the two diffusion weighting periods. This is done to consolidate the seemingly contradicting results of [1] and [2] in a single numerical framework based on the theoretical work in [3-5].

MATERIALS AND METHODS

The MR signal acquired with a double wave vector weighting sequence was calculated numerically using a routine written in IDL (Research Systems, Inc., Boulder, CO, USA). We defined an ellipsoidal pore and modelled the random walk of a water molecule (using 1000 starting points randomly distributed in the pore) by calculating each new position with a pseudo random number distributed according to a 1d Gaussian for each cartesian coordinate. The width of the Gaussian was adjusted to obey the Einstein equation with a diffusion coefficient $D = 2\cdot10^{-9}$ m^2 s^{-1}. The time between evaluated particle positions was set to 0.25 ms. When hitting the pore wall, the remaining fraction of the displacement was used to jump at an arbitrary angle to a position inside the pore. To approximate an isotropic orientation distribution of the pores, we chose 1302 orientation vectors distributed regularly on the unit sphere. For each orientation and each particle path, the phase shift due to the four diffusion gradient pulses ($\mathbf{G}^{(1)}$, delay Δ, $-\mathbf{G}^{(1)}$, delay τ_m, $\mathbf{G}^{(2)}$, delay Δ, $-\mathbf{G}^{(2)}$) was calculated for different angles, θ, between the diffusion gradients. Rectangular gradient pulses of one time step duration (i.e. $\delta = 0.25$ ms) were assumed, relaxation effects were neglected. We then averaged the signal over all orientations of the pore relative to the gradients. Oscillations due to numerical inaccuracy were suppressed by averaging the results over angular ranges in θ of 10° width.

RESULTS AND DISCUSSION

As Fig. 1 shows, the numerical results successfully reproduce the shape of the MR signal dependence on the angle θ between the diffusion gradients as shown in [1] and [2]. According to [3], the signal from randomly oriented pores should depend on θ as $S(\theta) \propto 1 - c\,(k^2/3)\,(2+\cos\theta)$, with c dependening on the average pore size, if $k = \gamma\delta G$ is small and if the time lag between the onsets of the second and third gradient pulse is $\tau_m = 0$. For this calculation it is assumed that the mean time required for diffusion across a pore, τ_D, and the duration, δ, and separation, Δ, of the diffusion gradient pulses obey $\delta \ll \tau_D \ll \Delta$. In this case, the diffusion-induced signal loss should vary by a factor of 3 between parallel (largest attenuation) and antiparallel gradient orientations. Fig. 1a approximates this behaviour with a factor of 2.5. This effect is present for spherical pores. In the case $\tau_m \gg \tau_D$ however, the signal is lowest for perpendicular gradients, as can be seen in Fig. 1d. This effect will vanish for spherical pores (Fig. 1b). The simulations also show that both effects are diminished but still present at longer gradient pulse durations δ (not shown).

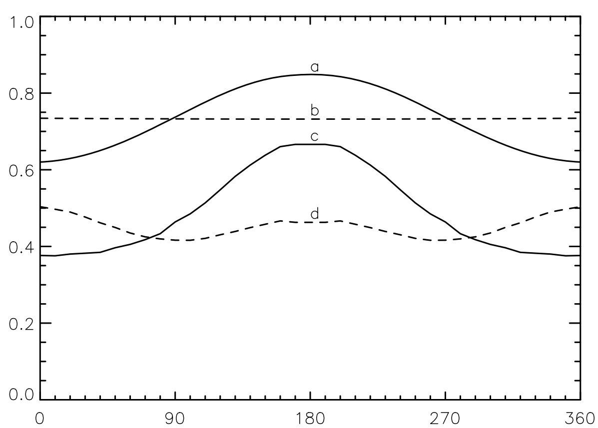

Fig. 1: Simulated MR signal (normalized) averaged over pore orientations, versus angle between gradients, θ (in degrees). For all experiments $\Delta = 250$ ms, gradient amplitude $G = 2$ T m^{-1}.
(a): spherical pore (radius = 6.5 µm), $\tau_m = 0$
(b): spherical pore, $\tau_m = 375$ ms
(c): elliptical pore (semiaxes 4, 4, and 20 µm), $\tau_m = 0$
(d): elliptical pore, $\tau_m = 375$ ms.

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