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Diffusion-Diffraction Phenomenon in multi-PFG experiments[1]

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Using pulsed-field-gradient (PFG) experiments, the sizes of the pores in ordered porous media can be estimated from the diffraction-like non-monotonic patterns that the signal attenuation curves exhibit [1]. A different diffraction pattern is observed when the experiment is extended to a larger number (N) of diffusion gradient pulse pairs as shown in Figure 1. When gradients of the same strength are applied along the direction perpendicular to the boundaries, diffusion pulse durations (δ) are small, and for extreme values of the diffusion times (Δ) and mixing times (t_m), the MR signal attenuation is given by

$$E_{\Delta=\infty,t_m=\infty}(\mathbf{q},N) = |S_0(\mathbf{q})|^{2N} \text{ , and} \tag{1}$$

$$E_{\Delta=\infty,t_m=0}(\mathbf{q},N) = \begin{cases} |S_0(\mathbf{q})|^2\,|S_0(2\mathbf{q})|^{N-1} & \text{, } N \text{ is odd} \\ S_0(\mathbf{q})^2\,S_0(2\mathbf{q})^*\,|S_0(2\mathbf{q})|^{N-2} & \text{, } N \text{ is even} \end{cases} , \tag{2}$$

where $S_0(\mathbf{q})$ is the Fourier transform of the pore shape function. For the N-PFG pulse sequence with arbitrary timing parameters (Δ, t_m and δ), the signal attenuation values can be computed using a matrix operator formalism [2].

Our simulations suggest that at long mixing times, the attenuation curves when $N > 1$ are similar to those from single-PFG experiments, but suffer more signal loss (see Figure 2a). However, when t_m is short, the attenuation curves from the N-PFG experiments are predicted to possess the following interesting features:

- When $N > 1$, the q-value at which the first diffraction dip occurs is exactly half of that for N=1. *This makes it possible to measure the sizes of* ***smaller pores*** (see Figure 2b).
- The qualitative differences between the N-PFG signal profiles for spherical, cylindrical and rectangular pores *may potentially aid in distinguishing between* ***different pore shapes***.
- For an even number of pulse pairs, the diffraction dips in the signal profiles are replaced by zero-crossings. Consequently, when there is a heterogeneous distribution of pore sizes, the effects of larger and smaller pores cancel each other maintaining the location of the signal loss at an intermediate value. *This makes it possible to estimate the average pore size even in porous media with a* ***broad distribution of pore sizes***. (see Figure 3).
- When N is even, the diffraction pattern is more resilient to decreasing diffusion times (Δ). *This makes it possible to measure the sizes of* ***larger pores****, helps avoid relaxation related signal loss, and reduces the total acquisition time* (see Figure 4).
- The diffraction pattern is relatively robust to small changes in mixing time. This is important because it may be difficult to satisfy the $t_m = 0$ condition when measuring smaller pore sizes.
- Similar to the case for $N = 1$, for longer diffusion pulse durations (δ), the diffraction dips shift towards the right making the pores appear smaller than they actually are.

We have investigated the diffusive diffraction phenomenon in multi-PFG experiments. The distinct features of the attenuation curves from the N-PFG experiments are predicted to yield significant improvements in the feasibility of acquisitions and widen the range of potential applications of the diffraction patterns. The achieved improvements may make the diffusive diffractograms used routinely for cell size measurements in clinical settings.

[1] A more comprehensive treatment of this work will appear in the Journal of Magnetic Resonance.

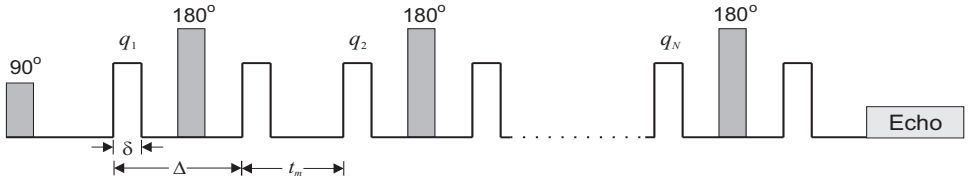

Figure 1: The N-PFG experiment. The gray boxes depict the RF pulses while the blank boxes show the gradients. All diffusion pulses have the same duration, δ. All N pairs have the same separation, Δ, and the consecutive pairs are separated by the same mixing time, t_m.

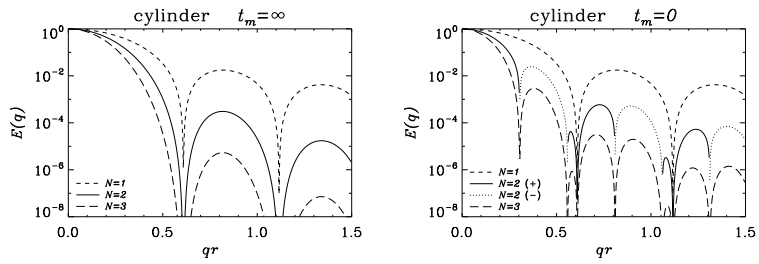

Figure 2: Signal with varying number of diffusion gradient pairs for a cylindrical pore with radius, r. $t_m \to \infty$ (left), $t_m = 0$ (right). In both cases, $\delta = 0$ and $\Delta \to \infty$. The dotted lines illustrate the negative sections of the $N = 2$ curve after flipping.

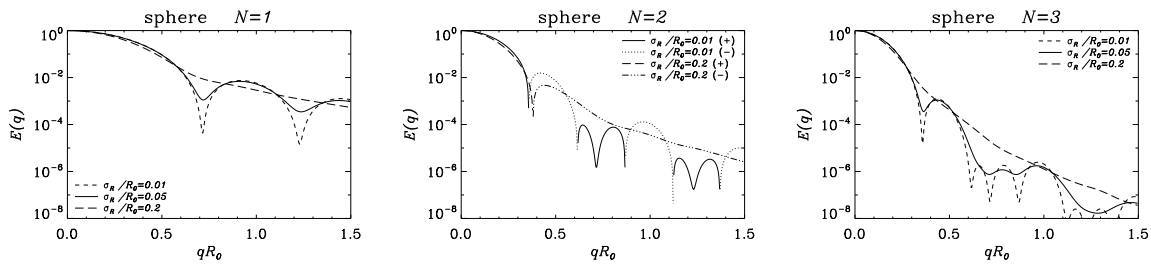

Figure 3: Signal attenuation curves as a function of q from distributions of spheres. The mean and standard deviations of the Gaussian-distributed radii of the spheres are denoted by R_0 and σ_R respectively. $\delta = t_m = 0$, $\Delta \to \infty$.

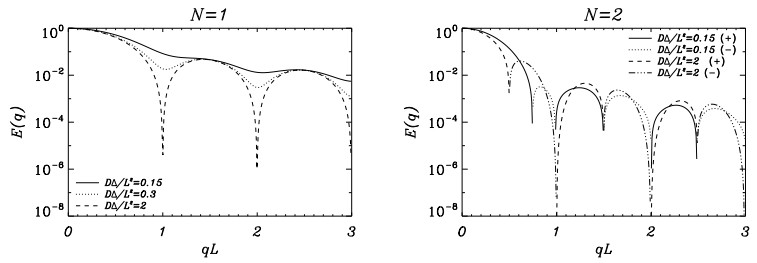

Figure 4: Signal with varying values of Δ for the parallel plane pore ($\delta = 0$, $t_m = 0$) with one (left) and two (right) pairs of pulses.

References:
[1] P. T. Callaghan et al., Nature, 1991, 351, p.467-469.
[2] P. T. Callaghan, J Magn Reson, 1997, 129, p.74-84.

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