Diffusion at Short Time Scales: q-space Imaging with Chirped Gradient Waveforms

A. J. Kiruluta[1,2], and I. A. Qasmieh[3]

[1]Physics, Harvard University, Cambridge, MA, United States, [2]Radiology, Massachusetts General Hospital/Harvard Medical School, Boston, MA, United States, [3]Physics, university of massachusetts Lowell, Lowell, MA, United States

Abstract: The practical limitations imposed by the requirement for delta function type diffusion sensitizing gradients in q-space imaging of diffusing spins, can be relaxed if these impulse gradients are replaced with chirped waveform gradient in a Chirp Gradient Spin Echo (CGSE) experiment. In this abstract, chirped diffusion sensitizing gradients are analytically and through numerical simulations and experiments, shown to yield a practical alternative that asymptotically approaches that using delta functions in a q-space experiment. In the measurements of temporal spectra, the chirped diffusion sensitizing gradients offer a practical alternative to the oscillating gradient spin echo experiment (OGSE) as well, where the apparent diffusion coefficient of the fluids can be measured in the short time regime in the presence of non-uniform restrictions. It is these restrictions that generate a dispersion of diffusion times resulting in a spectrum *D(w)*. The analytical expression for the b-value of the CGSE is derived and shown to be equivalent to that of the conventional pulsed gradient spin echo (PGSE) in the limit of zero chirp rate. Here we show for the first time that a CGSE sequence provides a practical sampling of the diffusion spectrum at conventional imaging gradient strengths levels. This is achieved by restricting the diffusion sensitizing power to the relevant diffusion spectral range, unlike the PGSE approach whose power is always concentrated in the low frequency range of *D(w)*.

Methods: In the restrictive diffusion case, the Fourier spectrum of the confinement space appears explicitly in the measurement, an effect which has been termed diffusive diffraction. One of the obstacle in PGSE q-space diffraction experiments concerns the reliance of the scattering formalism on an approximation of the gradient waveform by two narrow pulses. In particular, it is assumed that not only is the duration of the pulses much smaller than their separation ($\delta << \Delta$) but that the distance diffused during the pulses is small compared with characteristic dimensions of the pore morphology ($a < \delta$). Because the q wave vector amplitude depends on the time integral of the pulse, bounded by the available gradient power, this restriction to short pulses represents a constraint on the maximum available scattering wave vector and hence resolution. A successful analytical treatment of the finite pulse problem was demonstrated by Caprihan et al. [2] using a product of matrix operators approach. They showed that the PGSE consistently underestimates the pore size and concluded that the finite gradient pulse width effectively changes the resultant pore shape, making the isolated pores appear smaller than their actual size. By changing the chirp rate in a CGSE experiment, as shown in Figure 1, we found that the position of the first minima oscillates around the value *qa* (wave number *q* and pore size *a*) as shown in Figure 3 till a resonant frequency encoded in *D(w)* by the restrictive morphology approximates the embedded pore dimension at *qa*=1.

The physical origin of the effect of finite gradient pulse width on diffraction measurements for fluids in restricting geometry was also studied by Mitra and Halperin [3]. They used the concept of center of mass (*COM*) distribution function which is the spatial probability distribution of the center of mass of Brownian trajectories confined in a pore size of dimension *a*. Mitra and Halperin derived an analytical relation for COM distribution function and found that the root mean square width shrinks with increasing gradient pulse duration time or the isolated pore size appears smaller for larger pulse width. In this example of isolated pores and finite PGSE gradient pulse width, the COM of random walk distribution function piles up at the center of the pores, thus making the pores effectively smaller. In the limit of very long pulses, the walk during the pulse width uniformly fills the pores space, and COM is confined to the center of mass of the pore, or the effective pore size effectively shrinks to zero. However, in the case of chirped weighted COM using the CGSE gradients, the COM distribution is relaxed and spreads out towards the space of the pore in an oscillating manner around the true pore size as the sensitizing frequency approaches the inverse of the average step time.

Results:

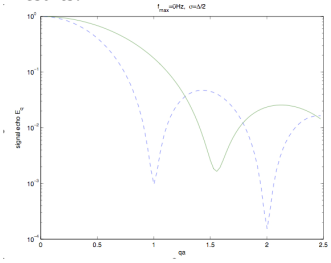

Figure 2

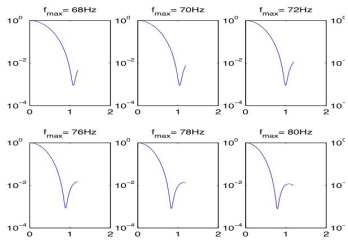

Figure 3

Figure 2 shows the signal echo of a PGSE experiment plotted against the wave number *qa*. The solid line shows the shift of the first minimum due to the finite pulse width while the dashed curve is the theoretical attenuation for an infinitesimal width gradient pulse ($\delta \to 0$). This graph clearly shows how the PGSE experiment underestimates the underlying pore size which it shift to a wave number *qa*=1.5.

Figure 3: Shows the oscillation of the first minimum in the diffraction pattern of the signal echo around *qa*=1 using the chirped waveform gradient for different chirp rate (f_{max}=68-82 Hz), and fixed gradient duration time. The horizontal axis represents the product of the *q* vector with the pore size *a*, while the vertical coordinate represents the signal echo amplitude. This result shows that sweeping the gradient frequency achieves the proper pore size parameter at f_{max}=72 Hz (*qa*=1)as we would expect in the theoretical implementation with a delta function diffusion sensitizing gradient. This pore size approximation oscillates from its true value sinusoidally so that within a chirped bandwidth, the true pore size value can be found at the resonant frequency.

Conclusions:

We have proposed a novel diffusion probing method using chirped gradient waveforms derived from a spectral interpretation of the diffusion process and verified the method analytically, through simulations and experiments. The analytical expression of the b-value for the chirped method was derived and showed to give the exact result as a OGSE experiment when the chirp rate is set zero.

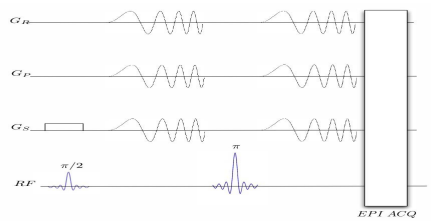

Figure 1: Timing diagram of diffusion sensitizing sequence showing the chirp gradient waveforms that are designed to encode the diffusion spectrum. The frequency sweep of the chirp is tailored to the underlying diffusion spectrum D(w) imposed by the restrictive morphology being imaged. The consequent reduction in diffusion probing power inherent in CGSE is overcome with the proposed MCGSE encoding scheme which is shown to be tunable to any desired diffusion spectral bandwidth such that: $G(t) = g(\omega_0 + 2\pi\kappa t)\cos\left(\omega_0 t + \pi\kappa t^2\right)/\omega_1$ with chirp rate $\kappa = (\omega_1 - \omega_0)/2\pi\delta$ and chirp duration δ is the chirp.

It was shown that using the CGSE diffusion gradients at a specific chirp rate, determined by the underlying pore geometry, makes it a practical alternative to the ideal delta-function pulse gradient, where the effect of the first dominant positive lobe in the CGSE gradient spectrum represents a PGSE sampling function of the diffusion spectrum *D(w)* and the finite width of this lobe is compensated by the higher frequencies in the chirp. However, these higher frequency lobes are generated at ever decreasing diffusion sensitizing power which reduces the effective bandwidth of the probed diffusion spectrum. By spreading the available power to only the spectral range of diffusion spectrum *D(w)* being probed, CGSE provides an efficient and practical implementation of q-space techniques on a conventional scanner.

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