Imaging the pore density function by synergistic diffusion-diffractions

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Introduction. The diffusion-diffraction phenomena in NMR[1], which is observed in narrowly dispersed, coherently organized systems[1,2], is a unique reporter for compartment morphology. The diffraction patterns in single-Pulsed-Field-Gradient (s-PFG) MR experiments arise from the fundamental Fourier relations between the signal decay, $E(\boldsymbol{q})$, and the averaged propagator, $\bar{P}(\boldsymbol{R},\infty)$, and are in fact the power spectrum of the pore microstructure[1]. The averaged propagator reports on the maximum displacements in the system, thereby in fact reporting the compartment size[2]; however, for various geometries of similar restricting length scales, the propagators appear quite similar. By contrast, the pore density function, $\rho(\boldsymbol{r})$, is the direct spectrum of the pore structure and as such holds all the information on the compartment morphology including size and shape; however, in conventional s-PFG MR, this quantity is intractable. Recently, zero-crossings and negative diffraction patterns were predicted[3] and reported[4] in the double-PFG (d-PFG) MR methodology[5]. Here, we show that by synergistic application of the diffraction patterns of d-PFG and s-PFG MR, one can in fact obtain the pore density function. Thus, an image of the pore space is obtained, without performing traditional MR imaging.

Aims. Obtaining the pore density function from diffusion MR measurements and studying the microstructural information it conveys.

Methods. The expressions for the s-PFG MR signal decay suggest that[3,6] $E^{sPFG}(\boldsymbol{q},\Delta_{\to\infty}) = |\tilde{\rho}(\boldsymbol{q})|^2$, where the structure function $\tilde{\rho}(\boldsymbol{q})$ is simply the FT of $\rho(\boldsymbol{r})$. Fundamentally, the power spectrum $|\tilde{\rho}(\boldsymbol{q})|^2$ is in fact the FT of the averaged diffusion displacement propagator $\bar{P}(\boldsymbol{R},\infty) = \int \rho(\boldsymbol{r})\rho(\boldsymbol{r}+\boldsymbol{R})d\boldsymbol{r}$ which for fully restricted diffusion is in fact the autocorrelation function (ACF) of the pore space. The d-PFG MR signal decay was found[3] to be $E^{dPFG}(\boldsymbol{q},\Delta_{\to\infty}) = \tilde{\rho}(\boldsymbol{q})^2\tilde{\rho}^*(2\boldsymbol{q})$. When the signal decay of d-PFG is divided by the signal decay of s-PFG, the synergistic signal decay, $N(\boldsymbol{q})$, is simply $N(\boldsymbol{q}) = \frac{E^{dPFG}(\boldsymbol{q},\Delta_{\to\infty})}{E^{sPFG}(\boldsymbol{q},\Delta_{\to\infty})} = \tilde{\rho}^*(2\boldsymbol{q})$. The pore density function is then just the FT of $N(\boldsymbol{q})$. To test the possibility of obtaining the pore density function, s- and d-PFG experiments were performed on a Bruker 8.4T magnet equipped with gradient coils capable of producing 195 G/cm in the x-, y- and z-directions. Both s-PFG and d-PFG NMR spectroscopy experiments were performed on an ensemble of water-filled cylindrical microcapillaries (the nominal inner diameter was 23±1 μm) that were coherently aligned with their principal axis pointing at the z-direction, the direction of the external magnetic field. The diffusion periods were set to 110 ms, and the gradient durations were 4 ms; 80 q-values were collected with $|\mathbf{G}_{max}|$=800 mT/m, resulting in a maximum q-value of 1362 cm^{-1}.

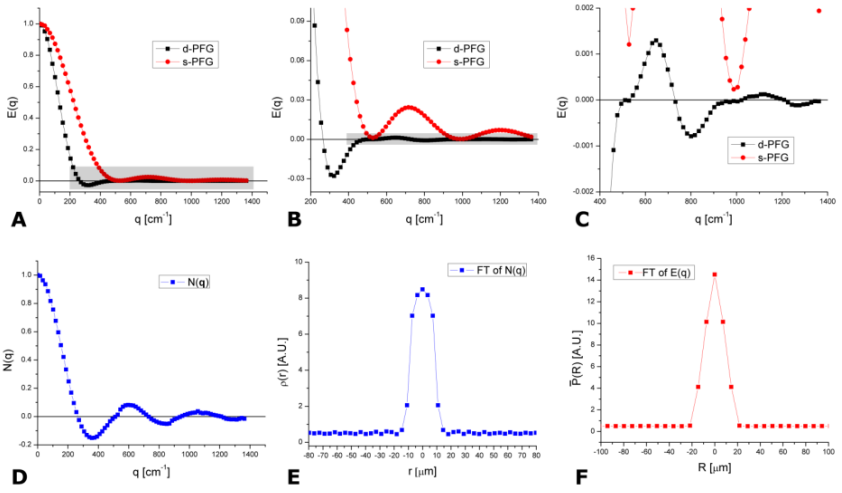

Figure 1. **(A)** Raw data for both s- and d-PFG MR experiments. **(B)** Enhancement of box in (A). **(C)** Enhancement of box in (B), showing the zero-crossings and negative diffraction patterns more clearly. **(D)** The $N(\boldsymbol{q})$ data, obtained by division of the two raw data signal. **(E)** The FT of $N(\boldsymbol{q})$, clearly yields $\rho(\boldsymbol{r})$, the pore density function. **(F)** The FT of $E(\boldsymbol{q})$ for s-PGSE MR data. The experiments were performed with long Δs and at the SGP regime.

Results and Discussion. Figures 1A-C show the signal decay in the s-PFG and d-PFG MR spectroscopy experiments. Note the marked diffusion-diffraction modulation for s-PFG MR, with the signal being constantly positive. The d-PFG MR signal exhibits the zero-crossings and consequently, the negative-diffraction patterns are obsevred[4]. Figure 1D shows $N(\boldsymbol{q})$ data, obtained by dividing the experimental data in the two individual experiments. Note how the signal oscillates between positive and negative values, and thus preserving the phase information that is conventionally lost in power spectra. Figure 1E shows the FT of $N(\boldsymbol{q})$. Indeed, a 1-dimensional projection of the cylindrical pore microstructure was directly obtained, i.e. an image of the pore density function, $\rho(\boldsymbol{r})$, was directly observed for the first time. The pore dimensions are in very good agreement with the nominal inner diameter, with the apparent radius being ~11 μm. Figure 1F shows the FT of the s-PFG MR $E(\boldsymbol{q})$ data, for comparison. Note that as expected, the triangular ACF of the pore space is obtained. The dimension of the pores can in fact be inferred from the base of the triangle since it describes the maximum displacement available in the system. Here, the maximum displacement is ~21.75 μm, in very good agreement with the nominal pore diameter. However, inherently, the fine details of the pore structure are lost, and very similar results would be obtained for pores having different microstructure. We then attempted to create a two-dimensional MR image based on $\rho(\boldsymbol{r})$ using back-projection of the $N(\boldsymbol{q})$ data (extrapolated to encompass twice as many zero-crossings as in the original data, to offer smoother images), via an inverse Radon transform (assuming cylindrical symmetry). The 2-dimensional image of the pore microstructure in the plane perpendicular to the principal axis of the pores that was obtained from $N(\boldsymbol{q})$ data is shown in Figure 2A. Note that this is an MRI image which directly describes the pore microstructure that was obtained without application of traditional imaging gradients. Figure 2B shows the 2-dimensional back-projection of the averaged propagator obtained from the FT of $E(\boldsymbol{q})$ data from s-PFG MR experiments. The fine details of the pore microstructure are lost due to the lack of zero-crossings, or phase information in the original $E(\boldsymbol{q})$ data. Note that the resolution of the images is dependent on the resolution in the q-axis. In the images shown in Figure 2, the in-plane resolution is 1.84x1.84 (μm)^2. However, acquiring the $N(\boldsymbol{q})$ data up to higher q-values using stronger gradients would yield even much higher resolution.

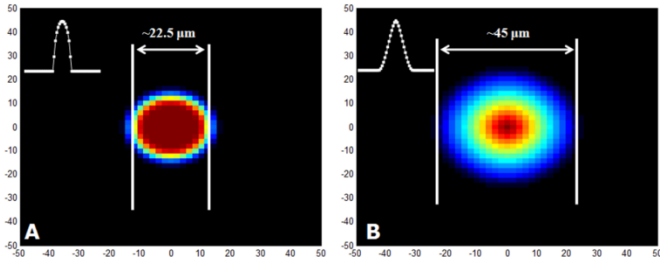

Figure 2. (A) Two dimensional back-projection of the pore density function obtained from $N(\boldsymbol{q})$. **(B)** Two dimensional back-projection of the averaged diffusion propagator obtained from $E(\boldsymbol{q})$. Clearly, the image of the cylinder in the plane perpendicular to its main axis is obtained only in (A). The in-plane resolution is 2 μm.

Conclusions. The pore density function was directly obtained from synergistic diffusion-diffraction patterns in d- and s-PFG MR.

References. [1] Callaghan et al., Nature **1991**, 351:497. [2] Cohen Y and Assaf Y, NMR Biomed **2002**, 15:516. [3] Özarslan and Basser, J. Magn. Reson. **2007**, 188:288. [4] Shemesh and Cohen, J. Magn. Reson. **2008**, 195:153. [5] Shemesh et al., NMR Biomed. **2010** 23:757. [6] Price, Concepts Magn. Reson. **1997**, 9:299.