Diffusion Pore Imaging by Double Wave Vector Measurements

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Introduction: In many porous systems, the main interest of NMR imaging is the determination of the shape of the pores, and not their position in the sample. Recently, two methods have been proposed to obtain the exact shape of closed pores by NMR diffusion measurements [1,2] by preserving phase information contrary to q-space imaging [3]. The signal can be collected from the whole sample enabling to measure an "average pore" with a higher signal-to-noise ratio (SNR) than in conventional NMR imaging. The first method [1] uses a combination of a very long and a short gradient pulse. The second method [2], which is considered here, relies on the application of short gradient pulses, which may be advantageous regarding sequence design. Here we show that the initial approach described in [2] is only applicable to point symmetric domains and present an extension to arbitrary domains [4,5].

Theory: Two measurements are used: A single pulsed field gradient (sPFG) q-space measurement with two short gradient pulses of duration δ and gradient vectors **G** and **-G** yielding $\mathbf{q} = \gamma\delta\mathbf{G}$ and a double PFG acquisition with three equally spaced gradient pulses **-G**, $2\mathbf{G}$ and **-G**. In the long time limit, the signal attenuations for sPFG and dPFG are given by

$$S_2(\mathbf{q}) = |\tilde{\rho}(\mathbf{q})|^2 \text{ and } S_3(\mathbf{q}) = \tilde{\rho}(\mathbf{q})^2 \tilde{\rho}^*(2\mathbf{q}), \qquad [1]$$

where $\tilde{\rho}(\mathbf{q})$ is the Fourier transform of the pore space function $\rho(\mathbf{x})$, which equals zero outside and the reciprocal pore volume inside the pore. Since $\tilde{\rho}(-\mathbf{q}) = \tilde{\rho}^*(\mathbf{q})$, it can be shown that $\tilde{\rho}$ is real exactly if $\rho(\mathbf{x}) = \rho(-\mathbf{x})$. Thus, for point symmetric domains, $\rho(\mathbf{x})$ can be directly obtained from the quotient of the two measurements (**method 1)**

$$N(\mathbf{q}) = S_3(\mathbf{q})/S_2(\mathbf{q}) = \tilde{\rho}(\mathbf{q})^2 \tilde{\rho}^*(2\mathbf{q}) \big/ |\tilde{\rho}(\mathbf{q})|^2 = \tilde{\rho}^*(2\mathbf{q}). \qquad [2]$$

However, for arbitrary domains the last part of the equation is not valid and we propose an iterative approach to recover the phase information from $S_3(\mathbf{q})$. We write $S_3(\mathbf{q}) = M(\mathbf{q})e^{i\cdot\varphi(\mathbf{q})}$ and $\tilde{\rho}(\mathbf{q}) = A(\mathbf{q})e^{i\cdot\psi(\mathbf{q})}$ and find using Eq. 1

$$A(\mathbf{q}) = \sqrt{S_2(\mathbf{q})} \text{ and } \psi(\mathbf{q}) = 2\psi(\mathbf{q}/2) - \varphi(\mathbf{q}/2). \qquad [3]$$

Since $\psi(0) = \partial\psi(\mathbf{n}\,q)/\partial q\,|_{q=0} = 0$ for the direction **n**, radial acquisitions of S_3 for different q-values can be used with appropriate interpolation to estimate iteratively the phase ψ and finally $\tilde{\rho}$ using S_2 (**method 2**). In principal, even measuring S_2 can be omitted, since $A(\mathbf{q}) = M(\mathbf{q}/2)\big/A(\mathbf{q}/2)^2$ and $1 - A(\mathbf{n}\,q) \propto q^2$ for small q can be used to iteratively estimate A (**method 3**).

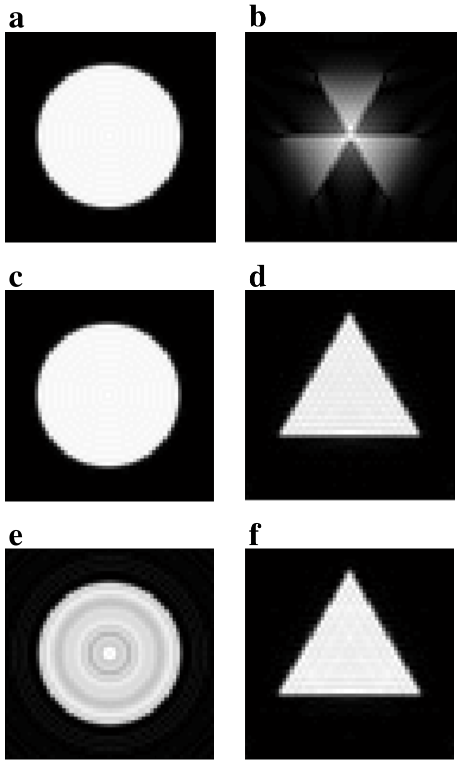

Fig.1: Reconstructed images; (a,b) method 1; (c,d) method 2; (e,f) method 3

Results: S_2 and S_3 were calculated using analytical expressions in the limit of long diffusion time and short gradients for 90 directions and 100 different q-values for a cylindrical and a triangular domain. To obtain the images, $\tilde{\rho}$ was calculated employing the three methods and an inverse Radon transform was applied (Fig. 1). While method 1 is successful for the cylinder (a), it fails for the triangular domain due to the lost phase information (b), since Eq. 2 is not valid. The estimation of the phase information using method 2 is successful for both domains. The pore space function can even be reconstructed using solely S_3 (e,f; method 3). Small artefacts in (e) result from the amplification of numerical errors in the iterative process of the estimation of A. Simulations with finite diffusion time (not shown) exhibit a faster convergence to the long time limit using the methods proposed here compared to the long-narrow gradient scheme suggested in [1].

Discussion: We have shown that it is possible to infer the exact shape of an arbitrary closed pore using short gradient pulses only. In contrast to the method proposed in [1], the methods using short gradient pulses allow using stimulated echoes, which may be advantageous to reach the long time limit, and they show better convergence properties. However, due to the iterative estimation process and the faster signal drop of S_2 and S_3 compared to $\tilde{\rho}$, the required SNR will be higher.

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