Localization regime of restricted diffusion in a model pulmonary acinus

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Purpose

A number of experimental and numerical MRI studies of restricted motion of spins diffusing in the human lungs have shown that the classical Gaussian approximation failed to describe correctly the signal attenuation, at least for relatively high gradients[1,2,3]. A better understanding of this discrepancy is certainly required for a quantitative NMR characterization of the alveolar tissue to diagnose lung diseases like emphysema. We performed numerical simulations for a model pulmonary acinus and found that the *localization regime*[4] of translational diffusion takes place. This new insight on the problem allowed us not only to explain a significant deviation from the classical exp(−bD) behavior, but also to quantify it more accurately.

Method

The internal morphology of the acinus was represented by different three-dimensional Kitaoka[5] labyrinths with a dichotomic branching structure filling the volume (Fig. 1). Emphysema representative geometries, created by random connections between different branches of the previous labyrinths, were also studied. Monte Carlo simulations of the reflected Brownian motion with one million particles were realized to compute the NMR signal[6]. An arbitrary acinus orientation in the chest was taken into account by averaging over all possible gradient directions in 3D space. A steady state gradient with different amplitudes g and durations T was applied to encode the diffusive motion of the nuclei of gyromagnetic ratio γ with a given free diffusion coefficient D, and the b-factor was $b=\gamma^2 g^2 T^3/12$.

Results and Discussion

A typical attenuation of the signal S as a function of g is shown in Fig. 2 (in this case, T=10 ms, D=1 cm^2/s, $\gamma=2.037894 \cdot 10^8$ rad $T^{-1}s^{-1}$). When g<2 mT/m, the Gaussian approximation $S \propto \exp(-bD_{app})$ was retrieved with an apparent diffusion coefficient D_{app} of about 0.16 cm^2/s, in good agreement with experimental observations[1,2]. For higher g, a stretch-exponential behavior $S \propto (bD)^{-1/6}\exp(-\alpha(bD)^{1/3}-\beta)$ with two parameters α and β was found, as for the localization regime in porous materials[4]. Similar results were obtained for emphysematic structures. This behavior could also be distinguished from the anisotropic diffusion model[2].

Conclusion

The signal attenuation as a function of gradient intensity in different 3D geometries representative of the healthy and emphysematic pulmonary architectures deviated from the isotropic and anisotropic Gaussian models. At high gradients (typically higher than 10 mT/m in our case), the localization regime model gave the best fit for numerical data. Changing the sequence parameters (e.g, timings, gradient profile), the stretched exponential behavior of signal attenuation as a function of gradient intensity could still be observed. These findings should be taken into account for future analysis of in vivo data.

References

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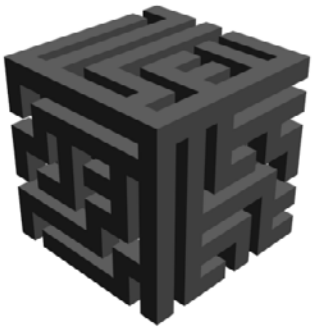

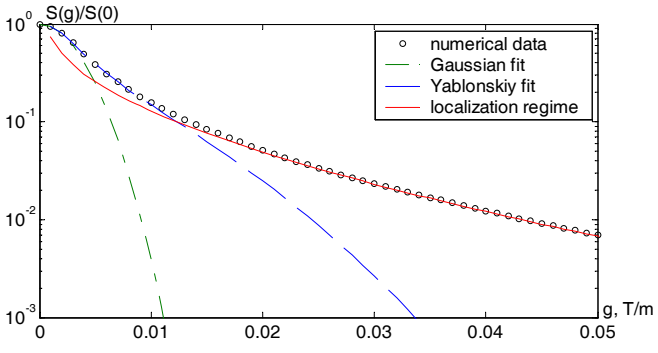

Fig. 1. (on left) Branching geometry of one realization of the model Kitaoka acinus of size 3mm composed of 6x6x6 cubic cells of 0.5 mm size.

Fig. 2. (on right) Comparison between the classical Gaussian approximation (D_{app}=0.16 cm^2/s), the anisotropic diffusion fit (D_T=0.01 cm^2/s, D_{AN}=0.49 cm^2/s), the localization regime behavior (α=0.385, β=0.2) and the numerical result for a typical signal attenuation in a model pulmonary acinus. Although the anisotropic diffusion fit looks good for g<12 mT/m, the values for diffusion coefficients D_T and D_{AN} are far from the expected ones[2]. In contrast, the apparent diffusion coefficient D_{app} is in good agreement with in vivo measurements[1].