Finite Element Simulations of ^{129}Xe Gas Diffusion in Models of Lung Airways

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Introduction

MR diffusion experiments using hyperpolarized noble gases are sensitive to lung microstructure [1-2]. Due to their very different free diffusion coefficients, ^{3}He and ^{129}Xe may be sensitive to different length scales of acinar structure. In this work, we investigate short-range ^{129}Xe diffusion in a model of acinar airways using finite element computer simulations. The results of these simulations are compared to previous ^{3}He diffusion numerical and experimental results; and their implications for the development of a quantitative theoretical model for lung morphometry based on ^{129}Xe diffusion MR are discussed.

Methods

Computer simulations were performed by solving the Bloch-Torrey equation using finite element method (Comsol Multiphysics). The geometric model consists of a central alveolar duct with branching nodes at both ends (Fig.1). The apparent diffusion coefficients (ADC) with gradients parallel (D_L) and perpendicular (D_T) to the central duct axis [3] were computed for a wide range of diffusion times (Δ= 0.5-6 ms) and gradient strength (G= 0-40 mT/m). The bulk ADC was obtained from the superposition of signals obtained for 91 uniformly oriented angular orientations of the gradient.

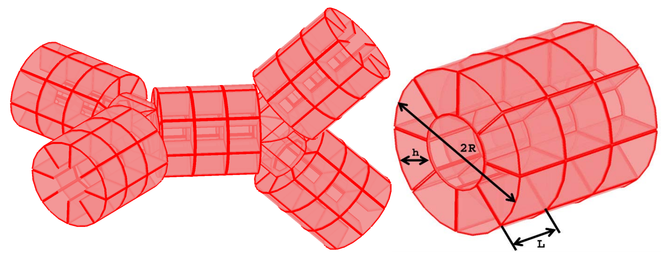

Figure 1. Geometric model of acinar airways: L=240 μm, R=350 μm and h= 200 μm.

Results and Discussion

Diffusion experiments can be represented as trajectories in a diagram that describes the interplay between length scales (diffusion length l_D, gradient dephasing length l_G, and structural length l_S) [4]. In Fig 2, trajectories corresponding to ^{129}Xe and ^{3}He experiments are shown, for structural lengths in the range found in acinar airways: l_S = 0.25, 0.38 and 0.5 mm. It can be appreciated that, while for ^{3}He at low G, diffusion is restricted for all three sizes; in the case of ^{129}Xe, only for the smallest structure is diffusion restricted. For the larger l_S, diffusion is free at low G.

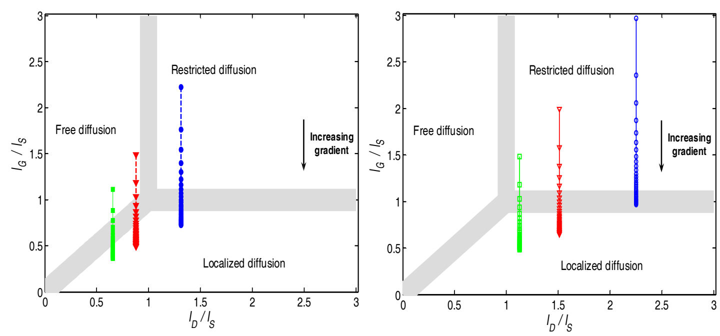

Figure 2. Diffusion diagrams for ^{129}Xe (left) and ^{3}He (right) gas mixtures, for structural sizes: l_S = 0.25 (circles), 0.38 (triangles) and 0.5 mm (squares).

These predictions are confirmed by the computer simulations, as shown in Fig. 3. For ^{129}Xe, there is a significant difference in apparent diffusivity between the intra and extra-alveolar spaces, while for ^{3}He, the differences in diffusivity are dominated by the distance from branching nodes. These results suggest that unlike ^{3}He, the ^{129}Xe diffusion signal may be modelled using a two compartment model (e.g. bi-exponential signal decay), with these compartments being physically distinct (i.e. intra and extra-alveolar space). This also suggests that ^{129}Xe diffusion MR may be more sensitive to alveolar destruction than ^{3}He, in agreement with previous predictions [5].

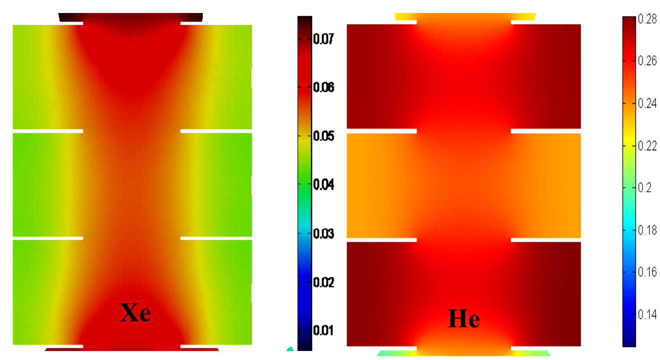

Figure 3. Distribution of diffusivities D_L (in cm^2/s) in the central duct for ^{129}Xe (in air, D_0= 0.14 cm^2/s. Δ= 4 ms) and ^{3}He (in air, D_0= 0.88 cm^2/s. Δ= 1.8 ms). Gradient oriented vertically.

From Fig. 3, it can also be appreciated that the reduced diffusivity of ^{129}Xe also makes branching effects less significant, which may help avoid some of the limitations that quantitative approaches, such as the cylinder model [1], face with ^{3}He. The cylinder model predicts D_L to decrease linearly with increasing b value for a broad range of diffusion times, but it has been demonstrated that ^{3}He shows a non-linear increasing behaviour for Δ> 2.5 ms [6]. ^{129}Xe shows a linearly decreasing D_L over a broader range of diffusion times (Fig. 4), which may significantly simplify the development of accurate theoretical models of ^{129}Xe diffusion.

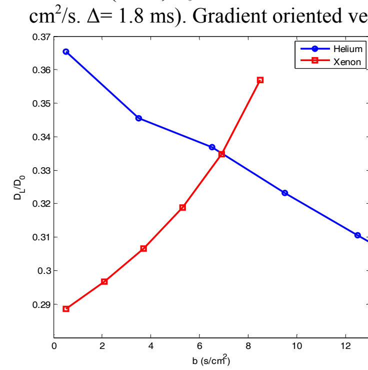

Figure 4. Longitudinal diffusivity as a function of b value for ^{3}He and ^{129}Xe for Δ= 4 ms. Unlike ^{3}He, ^{129}Xe still shows a linearly decreasing D_L for this diffusion time.

Conclusions

The numerical simulations presented here suggest that ^{129}Xe short range diffusion experiments may be more sensitive to alveolar structure than ^{3}He, while being less sensitive to branching effects. This may simplify the development of ^{129}Xe-based MR lung morphometry techniques, which could be based on a two compartment model rather than variants of the cylinder model.

References

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Acknowledgements

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