Simulating Helium-3 Diffusion in the Lung: Comparing the “Cylinder-Model” with Simulated 3D Alveolar Ducts

S. Fichele1, M. N. Paley1, N. Woodhouse1, Z. Sait1, P. D. Griffiths1, E. J. van Beek1, J. M. Wild1

1Academic Unit of Radiology, University of Sheffield, Sheffield, United Kingdom

Introduction: Devising a complete analytical theory that describes Helium-3 diffusion in lung tissue is difficult. The most recent attempt makes the approximation that each alveolar duct can be treated as a smooth walled, infinitely long cylinder, for which the diffusion equation can be solved [1]. In this case diffusion is considered anisotropic, and is categorized by two components; one along the principle axis, \(D_x\), and the other transverse, \(D_y\). The results from the transverse component can be used to predict the average radii of the alveolar ducts for which in-vivo experiments have yielded plausible results.

Here finite difference simulations have been used to model Helium-3 diffusion during a typical PSGE [2] experiment used in hyperpolarized gas imaging [3]. We simulated diffusion in 3D alveolar ducts using the model shown in Figure 1. The aim was to investigate how well the “cylinder-model” could estimate the radii of the simulated structures, given that they are not actually cylinders.

Methods: In brief, the magnetization was calculated at each node in a 3D grid using a finite difference method [3,4]. For each time step the phase of the magnetization was incremented according to the gradient strength at that position. A boundary wrapping technique was employed where magnetization at the periphery of the simulation volume could diffuse to the opposite side [3]. This eliminates boundary anomalies and allows diffusion to be investigated in infinitely long alveolar ducts. The 3D alveolar structures were generated from the loci of a cylinder, and 2

ADC values were calculated for a range of geometrical parameters, using \(b\)-values up to 10 cm\(^2\)s\(^{-1}\). Structures were systematically generated with fixed \(R_a\) and \(R\) while changing \(R_d\), from \(R-R_a\) to \(R+R_a\), e.g. Figure 2. For each individual structure, simulations were conducted for 30 gradient orientations from the principle axis \((0, 1/30 \pi, \ldots, 29/30 \pi)\). The results were then summed according to the “cylinder theory” [1] and the data then fitted to find an estimated value for the alveolar radius, \(R_{fit}\). This value was then compared to the effective radius of the structure, which was calculated as \(Reff = \sqrt{Volume/(\pi L)}\), where \(L\) is the length of the structure along the principle axis.

Results: A typical set of results, for a constant diffusion time (1.8 ms), are shown in Figure 3 for different gradient angles for the same structure. In Figure 4, the results from the same simulation have been summed according to the “cylinder model”, and then fitted to reveal an estimate value for the alveolar duct radius, \(R_{fit}\). The data fits well with the cylinder model trend, however, \(R_{fit}\) does not agree with \(Reff\). In Figure 5 the fitted radii for a set of simulations is compared to the effective radii for each simulated structure. The results demonstrate that \(R_{fit}\) doesn’t correlate linearly with \(Reff\) for ratios \(Reff / (R+R_a)\) below \(0.8\).

Conclusion: Finite difference simulations provide a good way of investigating diffusion in complex structures. We have demonstrated that the “cylinder-model” closely fits the results from 3D simulated alveolar ducts, however, the fitted data tends to overestimate the effective radii. Also, the estimation of radii does not necessarily correlate with the actual effective radius for structures where \(R_d\) is changing, i.e. in diseases like emphysema.

References