Microstructural analysis of foam-like structures by use of R2 dispersion

S. H. Baete[1,2], and Y. De Deene[1,2]

[1]Experimental Cancer Research, Radiotherapy and Nuclear Medicine, Ghent University, Gent, Belgium, [2]MR department, Ghent University, Gent, Belgium

Introduction

Quantitative Nuclear Magnetic Resonance (qNMR) research of in vivo microstructures is complex because many influences affect the measurable quantities. Insight in the underlying correlations of each of those influences is a necessary condition for the application of qNMR in determination of microstructure properties in vivo. Computer simulations can be used to determine these correlations. In this study a random walk simulation is presented to correlate the size of air cavities in foam-like structures with R_2-dispersion curves.

Materials and methods

The R_2-relaxation, caused by spin-spin interactions, in a restricted environment consists of several components [1,2,3]. Each of these components can be simulated using an extended version of a random walk implemented in Matlab. The relaxation due to internal field gradients can be derived by adding up the phase shifts a spin ensemble collects along its random journey. The internal field gradients caused by susceptibility effects can be determined with a magnetic field calculation algorithm [4]. The relaxation at the surface of the restrictive structures (surface relaxation R_{2S}) is implemented in the numerical model by attributing a specified loss of magnetisation at each collision with the surface

$$R_{2S} = \frac{1}{t}\ln\left(\frac{NP}{sumrelax(t)}\right)$$

where t is the diffusion time, *NP* is the number of random walkers and *sumrelax(t)* is the total amount of lost magnetisation during a time t. During a standard spin-echo sequence the random walkers in simulation are followed and at each time step data is collected.

The surfaces of the foam bubbles are implemented as a simplicial complex, that is, a union of triangles. To derive a foam-like structure in the simulation, a set of spherical bubbles (Gaussian spread radii) is randomly distributed in a voxel. The bubbles are then grown to air cavities with minimal energy surfaces using a gradient descent algorithm (Surface Evolver [5]) (fig 1). The triangulated bubble surfaces are then transferred to Matlab.

The random walk model is compared with gelatine foam. The gelatine foam is fabricated by dissolving gelatine (225 Bloom, type A, purchased from Sigma-Aldrich) [6% (w/w)] in de-ionized water [94% (w/w)]) at room temperature (approximately 22°C). After heating the gelatine solution to 45°C in order to obtain a sol and successive cooling down to 30°C, the gel is beaten by use of a household mixer. After approximately 1 min, a creamy white foam is obtained. The optimum time of beating the gel is determined on the basis of a visual inspection of the viscosity of the gel foam and the size of the bubbles.

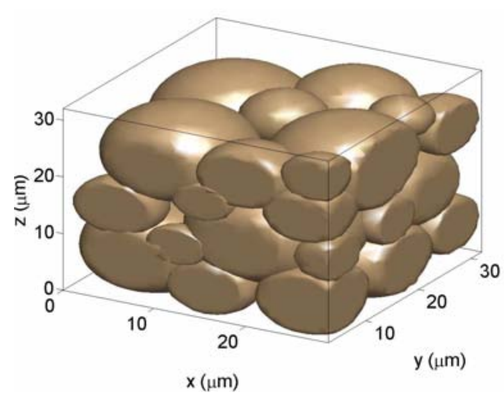

Figure 1: Foam structure obtained by Surface Evolver, mean radius r_0 5 ± 1μm, cut off at the planes x=29 μm and y=3 μm.

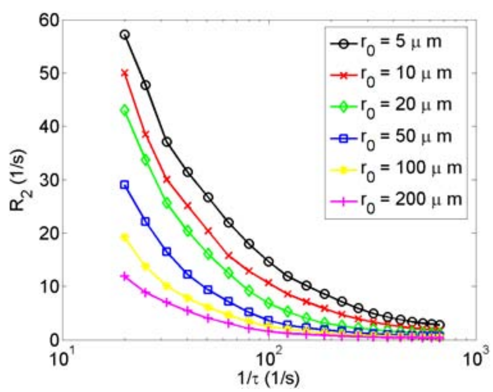

Figure 2: Simulation results (1000 random walkers, time step dt = 3.75 μs) of R_2-dispersion in foams with mean radius indicated and standard deviation 20% of mean radius. τ is half of the echo time.

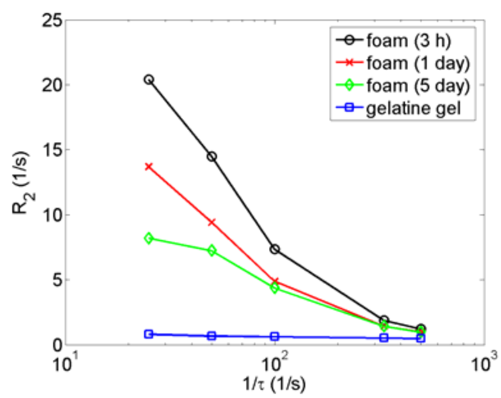

Figure 3: R_2-dispersion measurements of gelatine foam on different moments using a standard CPMG spin-echo-sequence on a Siemens Symphony 1.5 T scanner. τ is half of the echo time.

Results and discussion

The simulation results (fig 2) show the influence of mean foam bubble size r_0 on the simulated R_2-dispersion. R_2-disperion of the gelatine foam is measured on different moments in time (fig 3). Due to the coarsening effect in unstable foams, the mean bubble size of the gelatine foam increases over time [6]. The resemblance between simulation results and measurements permits estimation of mean foam bubble size and characterisation of the coarsening effect. From these results, it is clear that R_2 dispersion is a sensitive parameter that reflects the microstructure parameters such as foam bubble size.

Conclusion

The developed random walk simulation can be used to examine R_2-relaxation in media containing structures with surface relaxation and/or different magnetic susceptibilities. In this abstract the R_2-dispersion of a foam structure is simulated as an example. Simulations are in agreement with measurements. A computational quantitative approach of simple microstructures can lead to a greater insight in the relations between R_2-relaxation and microstructures. This study illustrates the applicability of R_2 dispersion for the determination of microstructure properties in lung tissue, e.g. the size of the alveoli. Future research should be conducted to implement this method for in vivo applications.

References

1. W.F.J. Slijkerman and J.P. Hofman, “Determination of surface relaxivity from NMR diffusion measurements,” Magn. Res. Im., vol. 16, pp. 541–544, 1998.
2. K. Dunn, “Enhanced Relaxation in Porous Media due to Internal Field Gradients,” J. Magn. Res., vol. 156, pp. 171–180, 2002.
3. A. Duh, A. Mohoric and J. Stepisnik, “Computer simulation of the Spin-Echo Spatial Distribution in the Case of Restricted Self-Diffusion,” J. Magn. Res., vol. 148, pp. 257-266, 2001
4. R. Bhagwandien, M.A. Moerland, C.J.G. Bakker, R. Beersma, and J.J.W. Lagendijk, “Numerical analysis of the magnetic field for arbitrary magnetic susceptibility distributions in 3D,” Magn. Res. Im., vol. 12, pp. 101–107, 1994.
5. K. Brakke, “The surface evolver,” Experimental Mathematics, vol. 1, no. 2 (1992), 141–165.
6. D. Weire and S. Hutzler, “The Physics of foam,” Clarendon Press, Oxford, 1999.