Monte Carlo simulations of transverse relaxation induced by superparamagnetic iron oxide nanoparticles with a semipermeable coating

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In nuclear magnetic resonance theory, transverse relaxation is caused by diffusion of the protons in magnetic field inhomogeneities. Indeed, that diffusion modifies the magnetic field experienced by each proton, hence their Larmor frequency, leading to progressive dephasing of their magnetic moments, and therefore to the transverse magnetization dropping to zero.

Therefore, when contrast needs to be introduced in the NMR signal, one way to do so is by adding magnetic material in the region of interest. Indeed, under the static NMR field, that material is magnetised, and therefore increases the magnetic inhomogeneity in the region of interest, which modifies the magnetization transverse relaxation time, and therefore the signal magnitude. For biomedical applications, a particularly suited contrast agent are superparamagnetic iron oxide nanoparticles, due to their low toxicity, high saturation magnetization, and null remnant magnetization [1].

However, for stability or functionalization reasons, those nanoparticles are usually coated with sugars, silica or polymers. Those coatings are usually semipermeable to water, in that water can usually penetrate the coating, but its diffusion is slower in there as compared with diffusion in the solvent. Because transverse relaxation is induced by diffusion in the field inhomogeneities, limited diffusion in the coating can be expected to impact relaxation times of water. Few experimental studies have analysed the impact of coating nature and thickness on relaxation time, but those who did hint to an effect indeed [2,3].

In this work, the influence of coating diffusion coefficient and thickness variations on transverse relaxation times of water in an environment loaded with coated iron oxide nanoparticles is probed, through Monte Carlo simulations. Nanoparticles are modelled as an impermeable sphere, which produces a dipolar magnetic field, surrounded by a semipermeable region, in which entry and exit of a proton is conditioned by coating permeability. Diffusion of the protons is modelled by a random walk, whose step is defined by the simulation time step and the diffusion coefficient in its environment.

References

1. Vuong, Q.L., Gillis, P., Roch, A. and Gossuin, Y. *WIREs Nanomed Nanobiotechnol.* 2017, **9(6)**, e1468.
2. Brero, F., Basini, M., Avolio, M., Orsini, F., Arosio, P., Sangregorio, C., Innocenti, C., Guerrini, A., Boucard, J., Ishow, E., Lecouvey, M., Fresnais, J., Lartigue, J. and Lascialfari, A. *Nanomaterials*. 2020, **10(9)**, 1660.
3. La Conte, L.E.W., Nitin, N., Zurkiya, O., Caruntu, D., O'Connor, C.J., Hu, X. and Bao, G. *Journal of Magnetic Resonance Imaging*. 2007, **26(6)**, 1634-1641.