Simulation of Water Nuclear Magnetic Relaxation Induced by Superparamagnetic Nanoparticles Trapped in a Biological Tissue

Éléonore Martin, Yves Gossuin, Quoc Lam Vuong
Service de physique biomédicale (UMONS)

The high-field T_2 relaxation of water molecules trapped in a biological tissue loaded with superparamagnetic iron oxide nanoparticles (SPIONs) is simulated using a Monte Carlo algorithm. The tissue is modeled as a periodic arrangement of semi-permeable membranes, and the influence of the membrane permeability on the relaxation is studied.

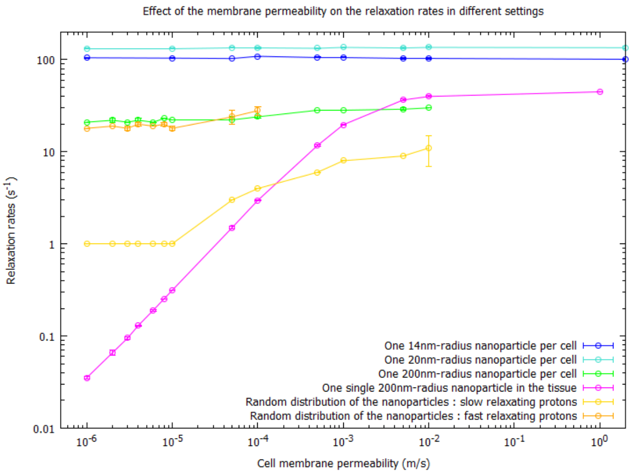
I. Context

- Various models describe the T_2 relaxation induced by SPIONs in an homogeneous medium.
- The diffusion of water molecules in the magnetic field inhomogeneities caused by the magnetic particles induces the relaxation [1].
- *In vivo* diffusion is constrained by cell membranes, which drastically affects the water diffusion coefficient D [2].
- This effect is too complex to be described analytically, but can be studied through Monte Carlo simulations.

II. Methodology: the algorithm

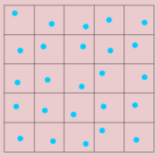
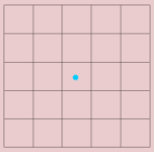
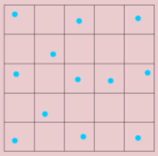
1. Generation of the simulation space, with its cubic cells and fixed nanoparticles.
2. Proton diffusion to a distance $\sqrt{6\,D\,\tau}$ where τ is the simulation time step. Upon meeting a membrane, the probability to cross it depends on the membrane permeability.
3. Dephasing of the proton magnetic moment depending on the magnetic field at its position.
4. Computation of the total magnetization at each time, and extraction of the system T_2 from an exponential fit.

III. Results, discussion and future prospects



Simulations of the effect of the membrane permeability in different settings, from [3]. The membrane permeability effect is stronger when the nanoparticle repartition is inhomogeneous.

Physical parameters : $B_{éq}$ = 0,16 T, 11x11x11 cells with a 10 µm side, diffusion coefficient D = 3 x 10^{-9} m²/s, f = 1,57 x 10^{-6}

Case	Results
	• No influence of the membrane permeability. • Can be explained by the symmetry of the system
	• Two proton populations (which tend to disappear at high permeabilities). → One corresponds to protons in loaded cells (with a *fast* relaxation) → One to protons in unloaded cells (with a *slow* relaxation)
	• High influence of the permeability when the nanoparticle distribution is inhomogeneous

Clearly, the impact of the permeability is not negligible and should be further studied. The model could be improved :

- by modelling the cells more realistically (in size and shape);
- by studying the effect of the aggregation of the nanoparticles in the cells which is experimentally observed [4];
- by adding the extracellular medium;
- …

---

[1] Q. L. Vuong, P. Gillis, A. Roch, and Y. Gossuin, « Magnetic resonance relaxation induced by superparamagnetic particles used as contrast agents in magnetic resonance imaging: a theoretical review », *Wiley Interdiscip. Rev. Nanomed. Nanobiotechnol.*, vol. 9, nº 6, p. e1468, November 2017.

[2] A. Szafer, J. Zhong, and J. C. Gore, « Theoretical Model for Water Diffusion in Tissues », *Magn. Reson. Med.*, vol. 33, nº 5, p. 697-712, May 1995.

[3] E. Martin, « Relaxation transverse de réseaux de cellules chargées de nanoparticules superparamagnétiques» (Master's thesis, 2018). UMONS, Mons, BE.

[4] L. Faucher, Y. Gossuin, A. Hocq and M.-A. Fortin, « Impact of agglomeration on the relaxometric properties of paramagnetic ultra-small gadolinium oxide nanoparticles », *Nanotechnology*, vol. 22, n°29, 21 June 2011.

BIOMEDICAL PHYSICS DEPARTMENT. Place du Parc, 23. B7000 Mons.
Contact : eleonore.martin@umons.ac.be