Numerical study of the distant dipolar field

S. Kirsch[1], and P. Bachert[2]

[1]Computer Assisted Clinical Medicine, Faculty of Medicine Mannheim, University of Heidelberg, Mannheim, Germany, [2]Dept. of Medical Physics in Radiology, German Cancer Research Center (DKFZ), Heidelberg, Germany

Introduction

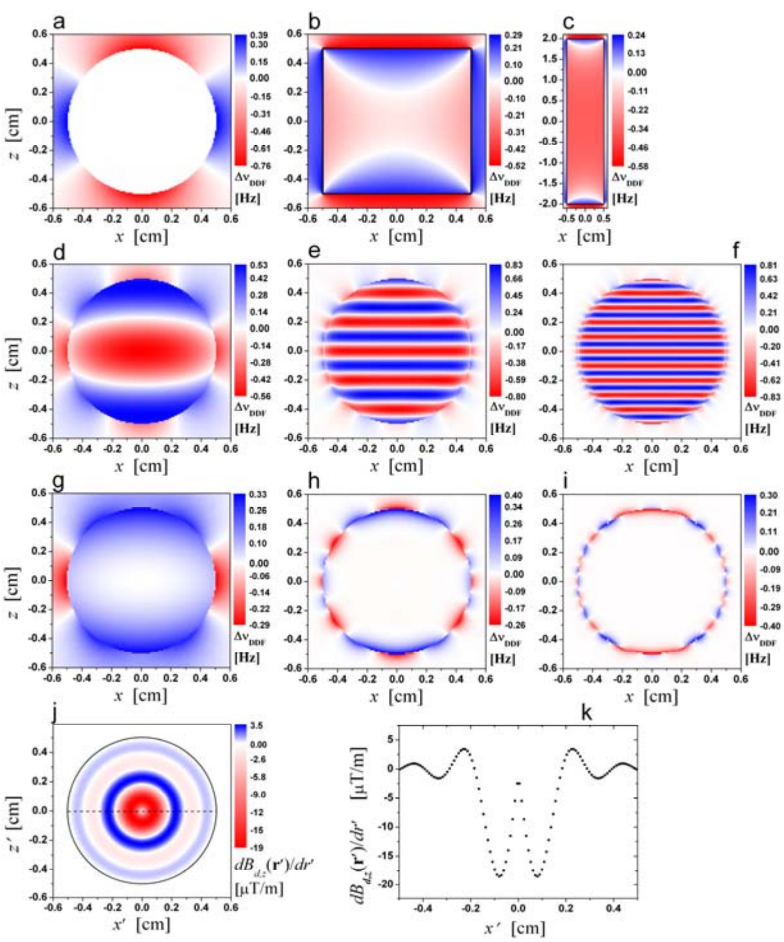
The direct action of the magnetic field generated by the macroscopic magnetization of a nuclear spin system in a static field $\mathbf{B}_0$ on the evolution of the ensemble was first observed and quantitatively understood in experiments on condensed ^{3}He by Deville *et al.* [1]. The results of these experiments could be explained by the presence of an additional classical magnetic mean–field generated by the macroscopic magnetization and "seen" by each spin in the sample. This so–called "demagnetizing field" or "distant dipolar field" (DDF) leads to similar effects in experiments on water at room temperature observed 11 years later by Bowtell *et al.* [2]. The DDF is given by

$$\mathbf{B}_d(\mathbf{r}) = \frac{\mu_0}{4\pi}\int_{-\infty}^{\infty} d^3r' \frac{3\cos^2\theta - 1}{2|\mathbf{r}-\mathbf{r}'|^3}\left[\mathbf{M}(\mathbf{r}') - 3M_z(\mathbf{r}')\cdot\mathbf{e}_z\right] \qquad (1)$$

where $\mathbf{e}_z$ = unit vector in the direction of the static field $\mathbf{B}_0 = (0,0,B_0)$, θ is the angle between the internuclear vector $\mathbf{r}-\mathbf{r}'$ and $\mathbf{B}_0$, μ_0 = vacuum permeability, $M_z(\mathbf{r}')$ = longitudinal component of the magnetization $\mathbf{M}(\mathbf{r}')$ at point $\mathbf{r}'$. The strength of the DDF depends on the geometry of the sample, on the thermal magnetization $\mathbf{M}_0$ and its spatial distribution. In particular, if the magnetization is modulated by a static magnetic field gradient (strength G, duration τ), the DDF is enhanced and exercises a significant influence on the temporal evolution of the spin system [1,2]. To our knowledge, pictorial representations of the DDF have been published for homogenously magnetized samples with spherical [3], ellipsoidal [4], and cylindrical [5] shapes. In this study, we performed numerical calculations to obtain 2D representations of the DDF in various geometries.

Material and Methods

The DDF was calculated by solving eq. (1) for each point of a 128×128 grid in the x–z plane. We assume perfect vacuum outside the samples and neglect susceptibility effects. Three different cases were considered: (i) cylinder and sphere homogeneously magnetized with $\mathbf{M}_0 = 0.02257$ A/m (H_2O at room temperature, spectrometer frequency = 300.1 MHz, *i.e.*, $B_0 = 7.01$ T), (ii) sphere with spatial magnetization distribution after the second rf pulse of the CRAZED–type preparation [6]: 90° pulse – z–gradient – 90° pulse, and (iii) sphere with the same preparation as in (ii) except the gradient is applied at the "magic angle" $\theta \approx 54.7°$. All integrations were done numerically by using the Maple® 11 software package on a PC equipped with 1 GB RAM and Intel Pentium® 4 processor operating at 3 GHz.



Results and Discussion

Figures (a–c) show the frequency offset $\Delta\nu_{\mathrm{DDF}}(x,z)$ due to the DDF for a homogeneously magnetized sphere with diameter $Ds = 1$ cm (a), cylinder with width and height of 1 cm (b) and cylinder with diameter of 1 cm and height of 4 cm (c). (d–f) Frequency offset $\Delta\nu_{\mathrm{DDF}}(x,z)$ resulting from the CRAZED–type preparation (ii). The wavelength of the magnetization helix $\lambda = 2\pi/(\gamma G\tau)$ was set to $\lambda = Ds$ (d), $\lambda = (1/5)Ds$ (e) and $\lambda = (1/10)Ds$ (f). (g–i) The same preparation as in (d–f), but the gradient is now applied at the "magic angle". (j) Illustration of the "correlation distance" $d = \pi/(\gamma G\tau)$. The derivative $dB_{d,z}(\mathbf{r}')/dr'$ gives the field contributions as a function of the distance that lead to DDF "seen" by a spin at the centre of the sphere. (k) Field contributions $dB_{d,z}$ per distance along the dashed line ($z' = 0$) in Fig. (j). Analysis of Figures j and k demonstrates that the most important contribution to the DDF at the centre of the sphere originates from magnetization in a spherical shell at a distance of 0.08 cm, which is in the order of the "correlation distance" $d = \lambda/2 = 0.1$ cm.

These numerical calculations show that the strength and the spatial structure of the DDF depend on the geometry of the sample and on the spatial distribution of the magnetization within the sample. The calculations verify a distance dependency. The main contribution to the total DDF originates from the magnetization within a spherical shell with *approximately* the distance *d*. This shell has a significant extension and therefore the correlation distance *d* should be considered as an average rather than an exact distance. Our results are consistent with the previous published 1D representation given in Ref. [6]. In the next step our simulation will be used to find spatial magnetization distributions which result in an enhanced DDF.

References:

[1] G. Deville *et al.*, Phys. Rev. B 19: 5666–87 (1979).
[2] R. Bowtell *et al.,* J. Magn. Reson. 88: 643–651 (1990).
[3] M. H. Levitt, Conc. Magn. Reson. 8: 77–103 (1996).
[4] T. Enss *et al.*, Chem. Phys. Lett. 305: 101–108 (1999).
[5] W. S. Warren *et al.*, Chem. Phys. Lett. 247: 207–214 (1995).
[6] W. S. Warren *et al.*, Science 262: 2005–9 (1993).