# Permanent Magnet Arrangements for Low-Field NMR

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**Abstract:** For low-field NMR, NdFeB permanent magnet arrangements are proposed to provide the static polarizing magnetic field. Especially a parallel and a circular arrangement of the permanent magnets, iron yokes and small shim magnets were tested and improved by COMSOL. The intent was to guide the design and the construction of NMR magnets by calculating the magnetic field strength and the associated field homogeneity for different arrangements, sizes and shapes of the permanent magnets and iron yokes, respectively.

**Keywords:** NMR, Magnetic Field, Permanent Magnet, NdFeB

## 1 Introduction

Nuclear magnetic resonance (NMR) studies with fluids contained in the void space of porous materials such as natural sediments (rocks, soils), cements, concretes, catalyst particles etc. are a modern non-destructive method in porosimetry(see e.g. [7] or [2]). In order to determine pore structure parameters such as porosity, pore size, fluid saturation and fluid-matrix interactions, representative sample volumes (a few ccm) of the fluid-saturated porous materials need to be introduced into a homogeneous magnetic field of relatively low magnetic flux density $(0,02 < B/\mathrm{T/m} < 0,2)$. For such studies, commercial NMR systems are often not well suited since they offer much too high magnetic flux densities and too small accessible sample volumes. Last but not least, purchase and operating costs for commercial magnet systems are generally high. Therefore, we designed two low-cost NMR magnets, which utilize modern NdFeB permanent magnets as source for the required magnetic flux. The NdFeB magnets are arranged together with iron yokes in such a way that a low but homogeneous magnetic flux density $B_0$ is generated over a large cylindrical sample volume (see figure 1). Simultaneously, these new magnet systems provide sufficient free space to access the samples enabling, e.g., NMR studies at high variable carbon dioxide and methane gas pressures, which are currently performed in our lab. A similar approach to low-field NMR was also described e.g. in references [1] or [6], where single-side magnets or different Halbach arrays were proposed.

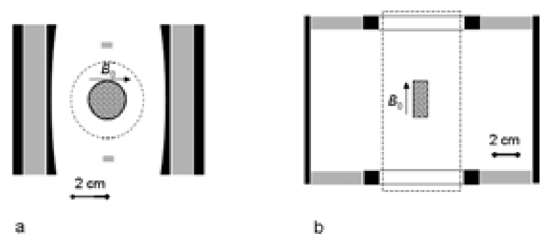


Figure 1: Sketches of the parallel (a) and the circular (b) arrangement of NdFeB magnets (gray) and iron yokes (black) for two NMR magnets. Sample volumes and access volumes (dotted lines) are indicated in the centers of both magnets.

## 2 Use of COMSOL Multiphysics

For NMR measurements a homogeneous magnetic field $B_0$ over the total sample volume is needed. Several different arrangements were tested as a model in COMSOL. The best suitable versions were chosen for further improvements of the field homogeneity.

In order to find the most homogeneous field, the profile and the lengths of the iron yokes and their distances were varied. The size of the NdFeB magnets were fixed since we intend to use commercially available permanent magnet bars. All problems are solved within COMSOL by magnetostatic models. The boundary condition "magnetic isolation" is set as shell much larger than the model. These shells of the models are a rectangle for the parallel arrangement and a cylinder for the circular arrangement.

The parallel arrangement (figure 1 a) is simulated by the 2D model "Perpendicular

Induction Currents, Vector Potential". The problem is split into two 2D slices perpendicular to each other. Each slice represents a cut through the center of the magnet arrangement.

$$\nabla\times(\mu_0^{-1}\mu_r^{-1}(\nabla\times A-B_r))-\sigma v\times(\nabla\times A) = A_z e_z \quad (1)$$

Investigations and improvements of the parallel arrangement (figure 1 a) started with the two parallel blocks of NdFeB magnets ($100 \times 100 \times 15$ mm$^3$ , $B_r = 1.3$ T). The minimum distance between them need to be $d = 51$ mm for the required access volumes in order to provide sufficient space for the experimental setup. Figure 2 shows the calculated deviations from the field in the center of the sample volume in this simple arrangement of two opposing permanent magnets.

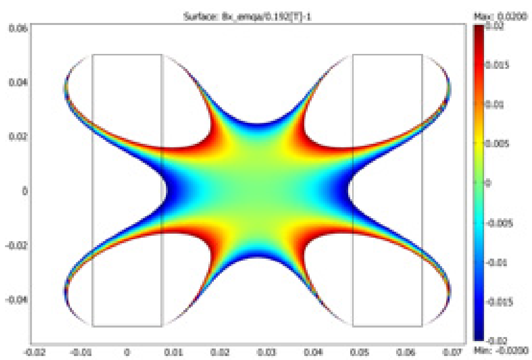

Figure 2: Residual relative magnetic flux of two NdFeB permanent magnets at a distance of 51 mm.

The first step to improve the homogeneity and to adjust the field strength was the addition of iron plates in front and back of each NdFeB magnet block (see figure 1). In the second step the inner iron plates were shaped. A Bézier curve consisting of 3 points was removed from a rectangle representing the inner iron plates. Two points were located at the corners of the rectangle and the last within the rectangle with equal distance to the other two points. This resulted in a bended surface (figure 3). To simplify the manufacturing, the Bézier curve used in the COMSOL simulation was approximated by a circle with a defined radius $r$.

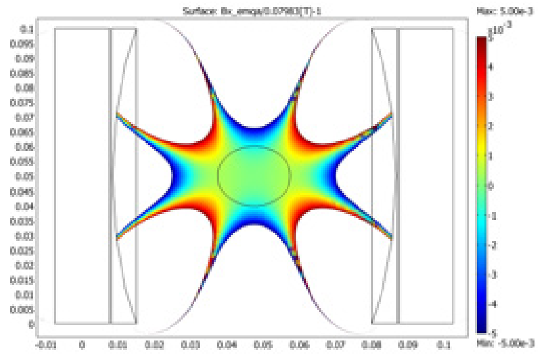

Figure 3: Residual relative magnetic flux of permanent magnets with shaped iron yokes.

Finally, the homogeneity of the magnetic field was further improved by adding shim magnets, which are composed of $2 \times 20$ small NdFeB cubes ($2 \times 2 \times 2$ mm$^3$) enframed with small iron bars at their pole faces.

The second 2D slice, which is oriented perpendicular to the slices presented in figures 2 and 3, shows two NdFeB magnet blocks located close to each other. This arrangement enlarges the area of the homogeneous magnetic field in axial direction of the cylindrical sample (figure 4). The repulsing force of the two magnets was calculated by COMSOL in order to find the minimum distance in between the two bar magnets on each side of the magnet. Additionally, it had to be investigated if iron yokes are able to bridge the gap between these two bar magnets and thus prevent inhomogeneities in areas where they are in close vicinity.

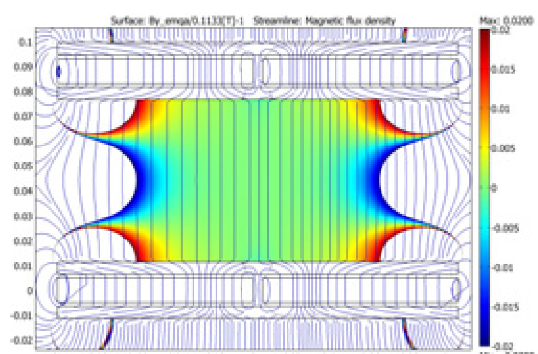

Figure 4: Residual relative magnetic flux in parallel arrangement, for four permanent magnet blocks. The sample position is in the center of this slice.

For the circular arrangement (figure 1 b) the 2D axial symmetry model "Azimuthal Induction Currents, Vector Potential"

$$\nabla \times (\mu_0^{-1}\mu_r^{-1}(\nabla \times A - B_r)) - \sigma v \times (\nabla \times A)$$

$$= (\mathrm{A}_{\phi,red} + A_{\phi,ext})e_\phi (2)$$

and the 3D model "Magnetostatics, No Currents" were used.

$$\nabla \cdot (\mu_0^{-1}\mu_r^{-1}\nabla V_m - \mathbf{B}_r) = 0 \qquad (3)$$

The magnet should be constructed out of two magnet stars each consisting of 16 NdFeB permanent magnet bars ($10 \times 10 \times 40\,\mathrm{mm}^3$) attached to an inner iron ring yoke. Both magnet stars are magnetically connected with each other at the opposite poles via 16 small bar-like iron yokes (see figures 5 and 6).

The value $B_r = 1.3\,\mathrm{T}$ was set to the residual magnetism and $\mu_r = 1.07$ to the relative permeability of the permanent magnets in the particular subdomains. No currents appeared in the model, so $v = 0$. For the subdomains of the yokes the predefined material "Iron" was used.

In the simplified 2D model (figure 5) the homogeneity was investigated and optimized by adjusting the lengths of the iron yokes. Then the 3D model (figure 6), with the optimized dimensions from the 2D model, yielded the correct field strength.

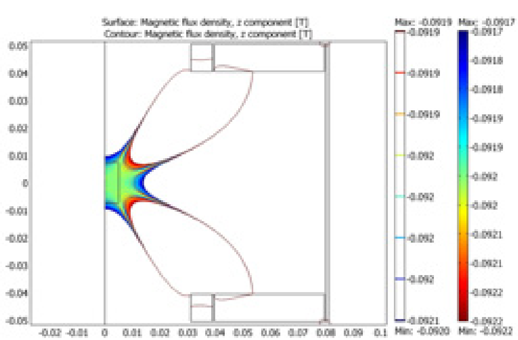


Figure 5: Magnetic flux in circular arrangement, 2D axial symmetry model. The sample position is indicated in the center of the figure.

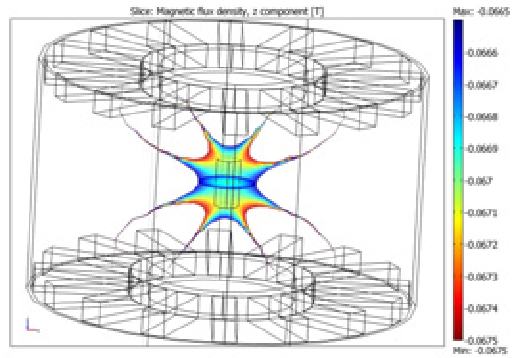


Figure 6: Magnetic flux in circular arrangement, 3D model. The sample position is indicated in the center of the figure.

In both magnet arrangements, the magnitude and the magnetic flux density at the sample position is of particular interest. Therefore, the mesh size in the sample region was generally chosen to be higher than in other regions. This was achieved by placing a cylinder with special mesh parameters in the center. The maximum element size was set to 0.002 m and the element growth rate to 1.5 at this subdomain. The finer mesh around the sample volume is shown in figure 7. Additionally, COMSOL was used to calculate the magnetostatic forces to find the appropriate supports for the mechanical design of the optimized magnet and iron yoke arrangements.

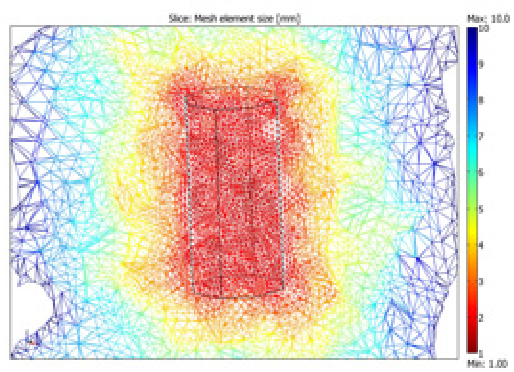


Figure 7: Mesh element size in the center of arrangement at sample position.

## 3 Results

In the parallel arrangement (figure 1 a), the best homogeneity of the $B_0$ field was achieved by using shaped iron yokes and small additional shim magnets. The investigation on the two NdFeB magnets alone showed an insufficient homogeneity (figure 2). At higher distances the homogeneity was even worse and the field strength $B_0$ decreased. Also the addition of iron plates of sizes larger than the NdFeB magnet blocks did not yield the desired magnetic field parameters. Such larger iron plates act like larger magnets with lower magnetic flux and the obtainable homogeneity is not sufficient for NMR applications.

The use of shaped iron plates improves the field homogeneity (figure 3). In the simulations, the curvature of the pole faces of the inner iron yokes was varied until the best homogeneity was achieved.

In order to achieve a homogeneity, which is sufficient for low-field NMR applications, the design needs further improvements. Two additional iron plates were situated at the outside to enlarge the return path of the magnetic field and shim magnets were placed with reverse polarity into the field of the main magnets. The magnetic field return path of the shim magnets is used to adjust the homogeneity. These shim magnets have to be located outside the access volume and outside the radio frequency coil surrounding the access volume. Hence size, strength and position of the shim magnets were optimized. In addition the radius of the inner iron yokes had to be changed to a higher value than without the shim magnets. A radius of $r = 450\,\mathrm{mm}$ was found to yield the best homogeneity of the magnetic flux. The value of the magnetic flux in the optimized design was calculated by COMSOL to be $B_0 = 115\,\mathrm{mT}$.

The force between two permanent NdFeB magnet blocks forming one side of the final magnet increases strongly with decreasing distances. This force must be carried by the support. For a distance of 5 mm the repulsing force is calculated to be 215 N. This force can easily be handled by aluminum frames. Figure 4 shows the arrangement of two NdFeB magnets on each side of the parallel magnet design. Although there is a gap of 5 mm between the magnets on each side, a good homogeneity of the field is achieved by the addition of the iron yokes which bridge the gap.

The optimized parallel arrangement was constructed and NMR experiments were performed in order to prove the suitability for applications. In a first step, the calculated value of the magnetic field strength was checked by comparing it with the experimentally determined Lamor frequency.

$$\omega = \gamma B_0 \tag{4}$$

By equation 4 the magnetic flux may be calculated via the resonance frequency in the $^1$H NMR experiment, where $\gamma$ is the gyromagnetic ratio. This approach yields the magnetic flux of $B_0 = 118\,\mathrm{mT}$, which agrees very well with the simulation results.

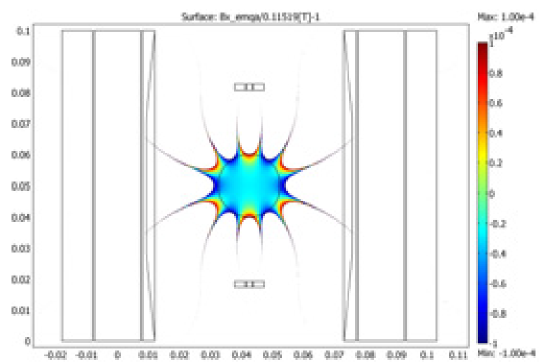

Figure 8: Residual relative magnetic flux in parallel arrangement.

Figure 8 shows the residual relative deviation of the magnetic flux density at the sample position for the optimized design. With respect to the field homogeneity, $^1$H NMR experiments with a water sample of 2 cm diameter and 3 cm length showed also good agreement with the simulation results. A monoexponetial fit on a primary spin echo decay ([3]) yielded a relaxation time of $T_2^* = 243\,\mu\mathrm{s}$. Via equations 5 and 6, the relative deviation of the magnetic flux can be calculated from these experimental result.

$$\delta\nu = \frac{1}{\pi T_2^*} \tag{5}$$

$$\frac{\delta B}{B_0} = \frac{\delta\nu}{\nu_\mathrm{L}} \tag{6}$$

The measured residual field inhomogeneity of $\frac{\delta B}{B_0} = 2.6\times10^{-4}$ (or 800 ppm) delivers nearly the same value as obtained in the simulation.

magnet design.

In order to simulate magnetic fields within COMSOL successfully, small gaps between materials with different magnetic properties need to be introduced. These gaps increase the size of the COMSOL models of the magnet arrangement, since COMSOL generates a large number of mesh elements in such gaps. This problem was circumvented by a two step procedure. First, a smaller model of similar geometry than the corresponding arrangement was simulated and the gap size was varied systematically until at an equal field strength and homogeneity a minimum number of mesh elements was achieved. Subsequently, this gap size was used in the full model of the magnet arrangement. E.g., for the shim magnets in the parallel arrangement, the optimal gap size between the small permanent magnets and the iron bars was found to be 0.3 mm.

Generally, the 2D models deliver already good solutions with important information regarding appropriate improvements of the magnet design. In the parallel arrangement, the shape of the magnetic field was derived by the two reasonably chosen perpendicular slices. The simulated magnitude and homogeneity of the magnetic flux density were found to agree well with the experimental values of the constructed magnet. For this arrangement, a 3D model, which would consume to much computer resources, proved to be not necessary.

For the circular arrangement, the 2D axial symmetry model was used to obtain first information on the optimum position of the NdFeB magnets and the lengths of the connecting iron yokes. However, it delivers a to high field strength since the local distribution of the 32 individual NdFeB magnets is not represented correctly. The final optimization of the arrangement was revealed by the 3D model. The best homogeneity in the 3D model is achieved if the distance between the iron yokes is reduced by only about 1 percent compared to the best homogeneity in the 2D model.

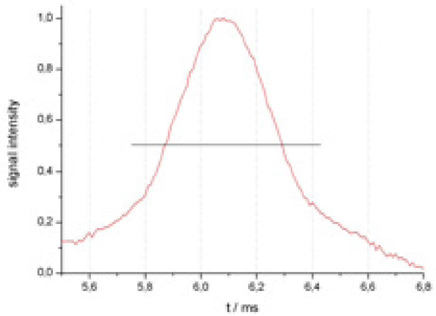


Figure 9: $^{1}$H NMR spin echo observed with a cylindrical water sample in the optimized parallel arrangement.

Other low-field NMR systems constructed of NdFeB permanent magnets, for example Halbach arrays, need a higher amount of permanent magnets and more space (see Raich and Blümler) [6]). The homogeneity of the magnetic field in a comparable sample volume is similar, but this is achieved by much higher effort in design an construction of the magnets. Hills ([5]) introduced a simple four magnet Halbach design ([4])and achieved a much lower homogeneity compared to our parallel arrangement (figures 1 and 8).

In the circular arrangement (see figures 1 b and 6) 32 NdFeB magnets were combined. The homogeneity was optimized by varying the length and the diameter of the iron yokes connecting the individual magnets. The outer diameter of yokes should be reduced to a minimum. Also the distance of the center and the return path between the upper and lower magnet stars were varied, but it showed no significant difference. Figure 6 shows the magnetic flux density in this arrangement.

## 4 Discussion

In order to handle the problems associated with limited computer resources on commercial computers, many simplifications had to be made to keep the COMSOL models of the NdFeB magnet arrangements at an acceptable size. The models only take materials with strong influence on the magnetic field into account. The support made of aluminum, brass and plastic was left out of calculations. Apart from assuming no influence, these materials were only used rarely in central areas of the

## 5 Conclusion

Simulations of magnetic flux densities are a useful approach in magnet system design for low-field NMR applications. The absolute values and the spatial variations of magnetic field predicted by COMSOL where found to agree very well with the corresponding quantities measured by NMR with the constructed magnets. Small differences between measurements with the constructed magnets and predictions by COMSOL result mainly from uncertainties in the manufacturing of the mechanical parts of the magnet.

Necessary simplifications in the COMSOL models have to be made carefully. Therefor the physics behind the model and the simplifications have to be taken into account and their influences on the result have to be rated by comparing different simulations and experiments.

## Acknowledgment

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