Simulation and optimisation of homogeneous permanent magnet for portable NMR applications

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***Abstract*— This paper focuses on the magneto static simulation of magnet arrangement used for portable NMR (Nuclear Magnetic Resonance) apparatus. In NMR experiments, a very homogeneous magnetic field is required in a large sample volume. In our case, NdFeB magnets are used to generate a homogeneous field, with a Halbach arrangement. The homogeneity of the magnetic field B_0 can be improved by dividing a long configuration of magnets into several rings. The size of useful volume is dependent on both the gap between each ring and some others shim magnets. Our aim is to enhance the sensitive volume size while maintain the highest magnetic field. In this goal, we optimized the gap between the two rings and put two shim magnets rings in the bore of the structure. Optimizing the position of the shim magnets allow drastic improvement. The homogeneity of the magnetic field B_0 is optimized with the help of CAD and mathematical software. Our results were confirmed with a Finite Element Method. As a result the method described here achieves a significant improvement of the homogeneity in the particular case of Halbach arrangement.**

Keywords-component; Nuclear Magnetic Resonance; Low field; portable permanent Magnet; Halbach; Shim magnets; Homogeneity simulation

I. Introduction

In recent years, Halbach type magnet has been developed extensively for use in a variety of applications [1, 2] because of their homogeneity and confinement of magnetic field inside the bore. Starting with the proposition of Klaus Halbach in 1980 [3], the Halbach ring consists of segments of permanent magnets put together in an array. This creates an homogeneous field in the transverse plane. Based on the principle of Halbach ring, the Halbach structure with discrete magnets for portable NMR known as NMR Mandhalas was given by Raich and Blümler [4]. It is based on an arrangement of identical bar magnets, described by the analytical equations reported in literature [5]. This concept has been widely used for building prototypes because they are easy to assembly and their region of interest is easy to access. The homogeneity of Halbach type is good in comparison to ex situ magnets, but poor compared to traditional non portable magnets [6]. For measurement of the relaxation times T2 and T1 or the spectrum, the inhomogeneity $\frac{\Delta B_0}{B_0}$ should not be higher than 10 ppm. T1 and T2 represent the relaxation of the nuclear spin magnetization, respectively parallel and perpendicular to the static magnetic field. To provide the sufficient field homogeneity for NMR experiments, a popular method is to add shiming magnets. The concept of movable permanent magnets in the shim unit of a Halbach array is reported by Ernesto Danieli et al [7]. Another method of shimming, based on the spherical harmonic expansion, proposes a complete procedure for permanent magnet design, fabrication, and characterization [8].

To understand the optimization of the placement of the principal magnets and of the shim magnets is the aim of this paper. We calculated and simulated the magnetic field B_0 and the homogeneity of a small NMR portable device with two rings of 12 magnets arranged in Halbach configuration. To improve the homogeneity of this device, we used eight shim magnets placed inside its bore. By optimizing the position of these magnets, we found out a configuration with a significant increase in the homogeneous region. These modeling and optimization were performed by Radia and Mathematica software, and confirmed by a Finite Element software (Ansys Multiphysics).

II. Materials and Methods

In most of the Halbach configurations, the static field B_0 is transverses to the cylindrical axis of the Figure 1. The direction of magnetization of each magnet is defined by two angles α_i and β_i.

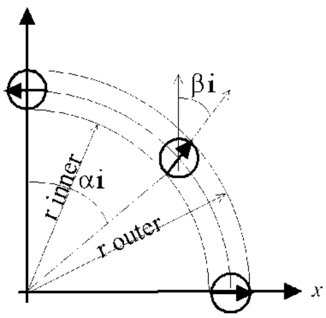


Figure 1. Geometric parameters of device

The i_{th} magnet is placed on a circle at an angle $\alpha_i = \frac{2\pi . i}{n}$ and its magnetization is defined by an angle $\beta_i = 2.\alpha_i$. Where n is the number of magnets (i = 0, 1, 2… n-1). Our configuration has 12 magnets placed on a circle of radius r_0 = 30 mm. As shown on Figure 2. - a, each magnet is placed at an angle $\alpha_i = i\frac{\pi}{6}$ and its magnetization is rotated by $\beta_i = i\frac{\pi}{3}$.

For compensation of the magnetic field outside of a ring, two others rings are placed in alignment as shown in Figure 2. and Figure 7.

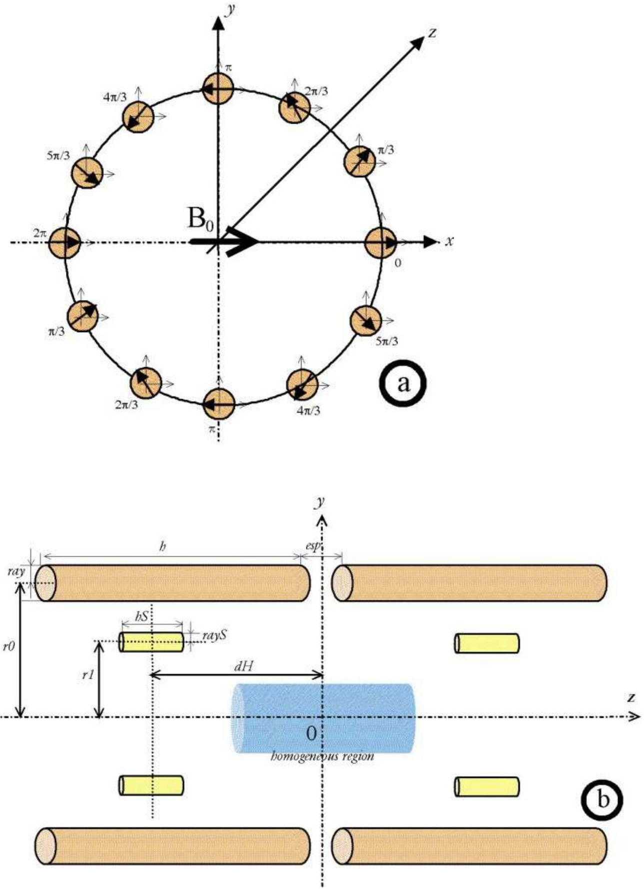


Figure 2. Position of magnets and their direction of magnetization

The geometric parameters of configuration are displayed in TABLE I.

To calculate the magnetic field of the magnet configuration, Radia [10] and Ansys [11] software were used. Radia was developed to design the Insertion Devices for Synchrotron light sources. It uses boundary integral methods. Each volume created to represent the magnets is subdivided in a number of sub-elements to solve the general problem of magnetization. The solution is performed by building a large matrix witch represents mutual interactions between the objects.

TABLE I. GEOMETRIC PARAMETERS OF OUR CONFIGURATION

Names of the parameter	Definitions	Dimensions
r0	Radius of the ring	30 mm
h	Height of the ring	50 mm
ray	Radius of magnets	4 mm
hS	Height of shim magnets	6 mm
rays	Radius of shim magnets	2 mm
esp	Gap between two rings	to be optimized
r1	Radius of the shim rings	to be optimized
dH	Distance from the middle length of shim magnets to z = 0	to be optimized

Ansys is a multiphysics software and it uses FEM (Finite Element Modeling) modeling. Each volume is divided with sub-elements. Even the air between and around the magnets has to be meshed. Flux conditions have to be placed outside the global volume in order to apply parallel or normal condition. Usually, boundary integral method is considered faster than FEM method. These two methods are used complementary: Radia is used for optimization because the simulation is faster than with Ansys. Ansys is used for verification of the results. The size of the meshing is reduced until the simulation results does not change.

The properties of the material that represent magnets during simulation were chosen to represent magnets from [12]. The magnet material is Neodinium NdFeB with a saturation magnetization of 1.37 T and with a coercitivity H_c = 1000 kA/m. The diameter and the length of the magnets are respectively 8 mm and 50 mm. The magnetization is oriented along the diameter. The maximal operating temperature is 120 °C and the temperature coefficient is 0.11 %.°C^{-1}.

In order to calculate the homogeneity, the values for the magnetic field are selected in the homogeneous region and treated by Matlab Software. The homogeneity is calculated by the formula (1).

$$Homogeneity = \frac{\sum_i^n \frac{Abs(B_i - B)}{B} 10^6}{m} \quad (1)$$

Where,

- B_i is the value of magnetic field at the ith position in the homogeneous region.

- B is the magnetic field value at the center of the homogeneous region.

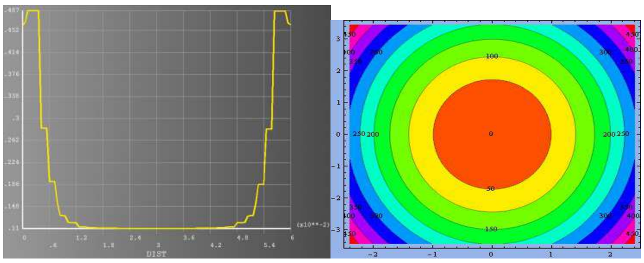
- m is the number of mesh nodes in the homogeneous region.

III. RESULTS

A. *Optimization of the gap between two rings without shim magnets*

A NMR device constituted with 24 magnets placed as shown in Figure 7. is considered during the simulation with Ansys and Radia. The magnetic field B_0 is oriented along Ox axis. First, *esp = 0* is considered. The maximal value of B_0 calculated with Radia is 0.103 T while the correspondent value derived from Ansys Analysis is 0.11 T. The difference of calculation between Radia and Ansys is 6.79 %. This difference can be accounted for by the problem of mesh size convergence. It means that the results of fine meshes are higher than coarse meshes. Furthermore, the difference can be acceptable.

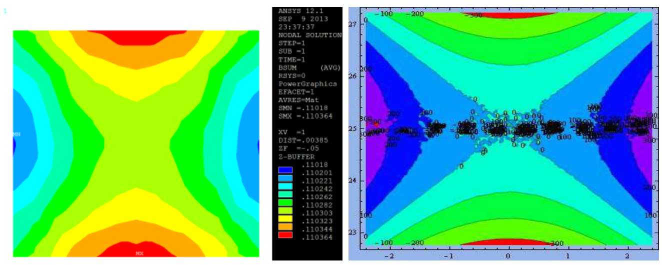
Figure 3. - a represents the variation of the magnetic field B_0 along the x axis; the value of the magnetic field is almost constant for 1.8mm < x < 4.2mm. Figure 3. - b represents the variation of the magnetic field B_0 in the plane xOy. Each shades of color represents a variation of the inhomogeneity $\frac{\Delta B_0}{B_0}$ of 50 ppm. In a rectangle of 5 × 6.4 mm, the inhomogeneity $\frac{\Delta B_0}{B_0}$ is larger than 450 ppm (Radia) and 380 ppm (Ansys). For an inhomogeneity lower than 100 ppm, the expected volume for experiment is 3 x 3 x 3 mm^3.



(a) Variation of magnetic field Bx versus x (b) Inhomogenity of the magnetic field Bx versus x and y

Figure 3. Magnetic Field Bx distribution at z = 0 (xOy plane)

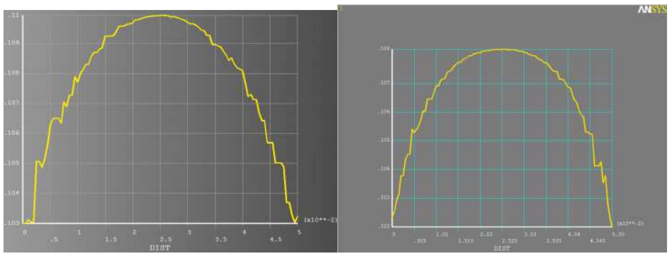
The variation of the magnetic field Bx on the xOz plane is shown on Figure 4. The homogeneity of magnetic field is 300 ppm in a region of 5 x 6.4 mm as determined by Radia, while Ansys gives a result of 200 ppm.



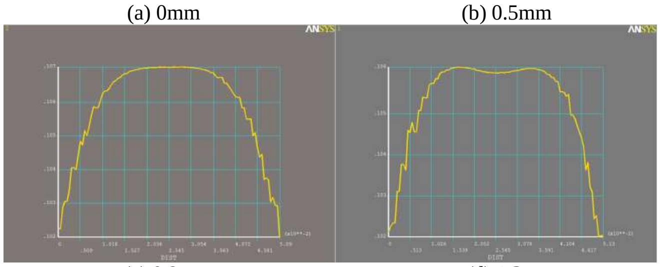
(a) Ansys result (b) Radia result

Figure 4. Magnetic Field Bx distribution in the region of 5 x 6.4 mm in xOz plane

The variation of the magnetic field Bx profile along Oz axis depends on the gap *esp* between the two rings. Best homogeneity is achieved at a certain distance. To optimize this gap, we increased the value of esp by steps of 0.1mm. Figure 5. shows Bx profile for four values of esp. When esp = 0, the magnetic field outside one ring does not compensate the magnetic field of the other ring. For esp = 0.9 mm, the compensation is optimum and the magnetic field at the center is almost constant.



(a) 0mm (b) 0.5mm



(c) 0.9mm (d) 1.3mm

Figure 5. The field profile at different distances

The useful volume for NMR sample is determined from the coordinates (x,y,z) of the point where Bx is maximal. Then, the volume is calculated with the 3 coordinates that generate a variation of $\frac{\Delta B_0}{B_0}$ not larger than 100 ppm. The Figure 6. shows that the volume of the homogeneous region is a function of the *esp*. The optimal value of esp determined by Radia is around 0.77 mm and the "useful" volume, is about 2640 mm^3. The volume is increased by a ratio of around 80 when the spacing between the two rings is optimized. This is caused by the decrease of the magnetic field outside one ring, which is similar to the other ring. There's an optimum gap between the two rings where the sum of the variations of the magnetic field outside the rings are canceled.

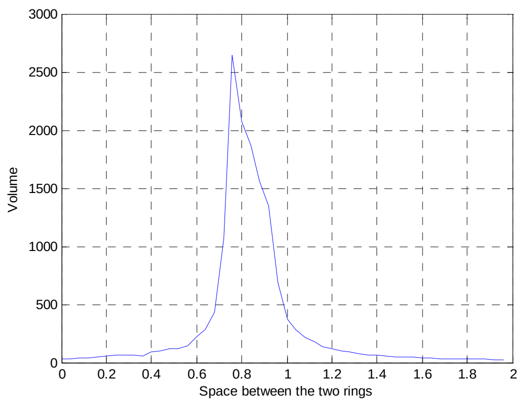
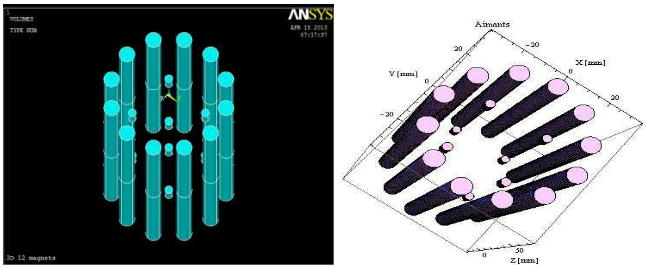


Figure 6. Volume of homogeneous region is a function of the gap *esp*

B. Optimization of the configuration with shim magnets

Although the magnetic field homogeneity increases by adjusting the gap between the two rings, the inhomogeneity of magnetic field also comes from magnetic material (dispersion in both the value and the orientation of the magnetization), errors in fabrication process and positions of the magnets in the array. These factors cannot be corrected by adjustment of *esp*. To overcome these difficulties, the shim magnets are considered as a way to compensate the inhomogeneity of the magnetic field [7, 8, 9]. In our case, we use eight small magnets placed inside the bore of the two rings as shown on the Figure 7.



(a) With Ansys (b) With Radia

Figure 7. Halbach magnets with 8 shim magnets modeled with Ansys and Radia

The direction of magnetization of the shim magnets is defined as shown in Figure 8.

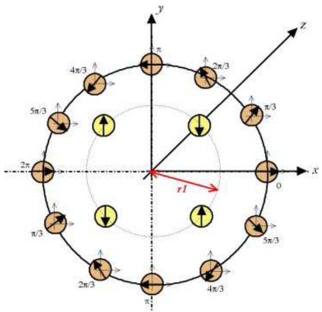


Figure 8. Direction of magnetization of the shim magnets

There are three variables that need to be optimized: *esp*, *r1* and *dH*. The optimization objective is to determine the values for *esp*, *r1* and *dH* that maximize the volume for a given inhomogeneity, in our case 100 ppm. The flow chart shown in Figure 9. describes the optimization process implemented with Mathematica concerning optimization and Radia for the calculation of the magnetic field. To avoid the superposition of the main magnets and the shim magnets, we set the range of *r1* from 15 to 23 mm and *esp* ranging from 0.1 to 0.6 mm. The optimal value for *esp* considered here is different from the value considered before because of the presence of shim magnets.

Each step of increase of *r1* is 1 mm while correspondent value of *esp* is 0.1 mm. Each possible values of *r1* are placed in a matrix. For all these values, the magnetic field and then the three coordinates x,y,z for an homogeneity lower than 100 ppm are determined. For each value of *r1*, a value for the volume is obtained. The value of *r1* that corresponds to the highest value of the volume is saved. The same process is repeated with *esp* and *dH*. After a variation of one parameter, the variation is refined around the best value previously obtained. It's very important to choose good initial conditions and begin the variation of one parameter with plausible value for the others parameters. This method was preferred to the use of Mathematica optimization functions, like *FindMaximum*.

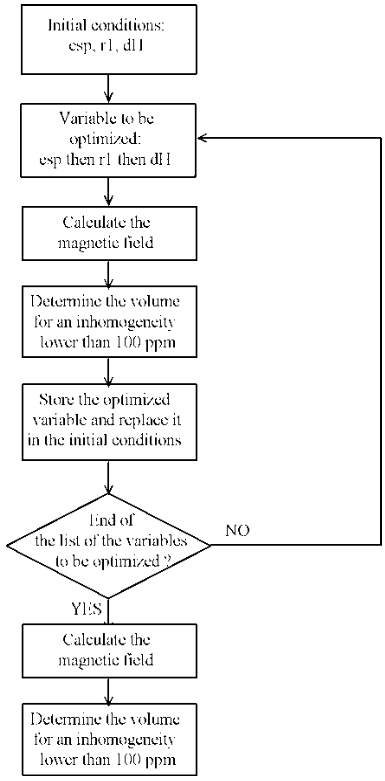


Figure 9. Optimum flow chart of our configuration with 24 main magnets and 8 shim magnets.

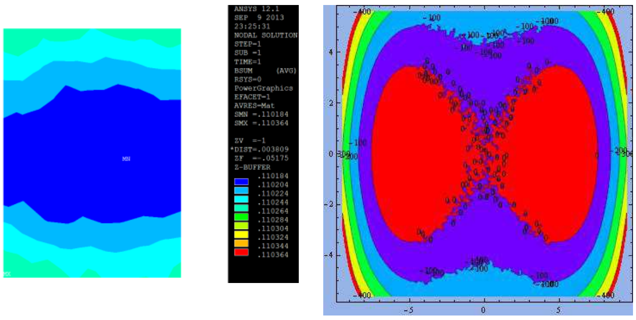
The optimum parameters are presented in TABLE II. :

TABLE II. GEOMETRIC PARAMETERS OF OPTIMUM CONFIGURATION.

Name of the parameter	Dimension
esp	***0.2 mm***
r1	***20 mm***
dH	***26 mm***

The optimization results give a great improvement of homogeneity, as can be seen in Figure 10. It shows that the inhomogeneity of the magnetic field calculated in a 7 x 8 mm region is 90 ppm after shimming while the value before shimming is 370 ppm.

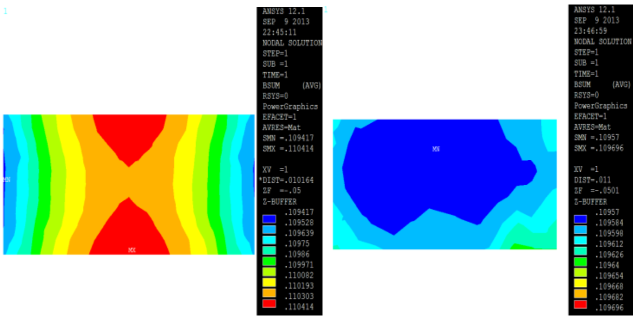
The magnetic field inhomogeneity calculated by Radia is in good agreement with Ansys. However, Ansys gives always smaller useful volumes than those obtained by Radia because of the method of calculation. This can be explained by the fact that the result from Radia is the highest value at the border of the region while the one that come from Ansys is the mean value for the overall region.



(a) Before shimming (b) After shimming

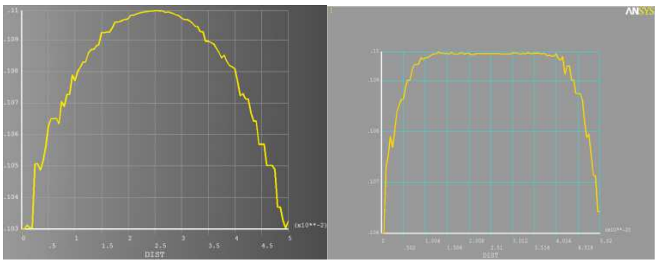
Figure 10. Magnetic field homogeneity in the xOy plane and z = 0.

The Figure 11. shows great improvement of homogeneity along z axis. The size of homogeneous region drastically increases in length from 8 mm to 25 mm. This is confirmed by the stability of the magnetic field profile of the Figure 12.



(a) Before shimming (b) After shimming

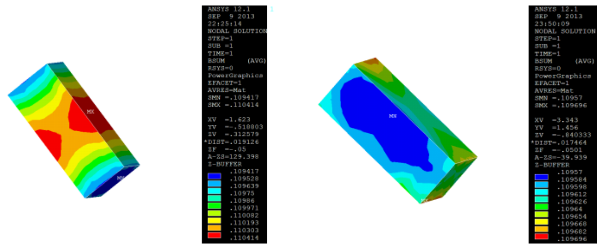
Figure 11. Magnetic field homogeneity in the region 8 x 20 mm along Z axis.



(a) before shim (b) after shim

Figure 12. Magnetic field profile at the center of the assembly of magnets.

The inhomogeneity of magnetic field in a volume of 7 x 8 x 20 mm is 230 ppm with the shim magnets in comparison to 4320 ppm in the case without shim magnets, as shown in Figure 13.



(a) before shim (b) after shim

Figure 13. Magnetic field distribution in the sensitive volume 7 x 8 x 20 mm^3 in 3D.

IV. DISCUSSION AND CONCLUSION

The study presented herein depicts two methods of simulation in order to determine the best achievable sample volume for NMR experiments. We described the optimization process of a light weight NMR portable device with two rings of 12 magnets that provide a magnetic field B_0 equal to 0.103 T. The study reported above, describes a process to calculate and simulate the magnetic field B_0 of a small NMR portable device in Halbach type and its homogeneity based on the Radia software. We verified those results with the finite element software Ansys multiphysics. The agreement of results between the two software is good. Based on the Radia and Ansys software analysis, we simulated the homogeneity of magnetic field and optimized the gap of two consecutive rings to increase the size of the homogeneous region. The optimum gap length is around 0.8 mm.

To compensate for the magnetic field inhomogeneity caused by the errors of fabrication process and dispersion of the magnetic properties of the magnets, we used eight small shim magnets placed at the center of the device. By optimizing the position of these magnets, the homogeneity significantly improves. The results of optimization show that the homogeneity for a given volume (7 x 8 x 20 mm) improves 18 times in comparison to the same configuration without shim magnets, with values lowering from 4320 ppm to 230 ppm. The homogeneity of region (7 x 8 mm) in transverse plane is 90 ppm while it is 370 ppm without shim magnets. This shim technique allows for the use of larger samples in NMR experiments. Before optimizing the gap between the two rings and the position of shim magnets, the useful volume for NMR experiments was around 33 mm^3. After optimization, the useful volume for NMR experiments is around 500 mm^3.

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