Optimization-based ambient field compensation applied to fast-field cycling nuclear magnetic resonance experiments

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***Abstract* — Fast-field cycling (FFC) nuclear magnetic resonance applications require compensation of the ambient magnetic field, which may be stated in terms of a multi-objective optimization problem involving the spherical harmonics decomposition of the compensation coils. In this article, this optimization-based approach is detailed and applied to the particular case of a FFC relaxometer.**

I. INTRODUCTION

Nuclear magnetic resonance (NMR) techniques are based on the interaction of matter and magnetic fields. In a typical NMR experiment, a sample is subjected to a combined sequence of static magnetic fields and radio frequency pulses that induces the forced precession of its nuclear magnetic moments [1]. The treatment and analysis of the electromagnetic signals detected during the experiment lead to various applications, which include NMR spectroscopy and magnetic resonance imaging (MRI). In traditional NMR techniques, the sample is submitted to field intensities much higher than the Earth's magnetic field. However, advances in NMR have shown that switching between multiple field levels during the experiment (*Fast-Field Cycling*, FFC) can provide valuable additional information on the sample composition (FFC-NMR relaxometry [2]) and result into improved imaging contrast and diagnosis (FFC-MRI [3]).

The range of field strengths swept in such approaches may include very low or virtually zero field intensities, making these experiments very susceptible to the disturbing ambient field. As a consequence, a compensation system capable of cancelling the Earth's magnetic field and other environmental disturbances while keeping a high degree of field homogeneity is required in this context of applications.

This article discusses how field compensation can be regarded as an optimization problem stated in terms of the spherical-harmonics decomposition of the total ambient field. The numerical scheme arising from this discussion is then applied to the particular case of a FFC-NMR relaxometer. As it will become clear, the proposed approach is well adapted to enforce the spatial field requirements imposed by NMR applications.

II. AMBIENT FIELD COMPENSATION

The total magnetostatic field $\mathbf{B}$ in a domain Ω free of internal electrical currents admits a scalar magnetic potential ψ. This potential is a solution of Laplace's equation $\nabla^2\psi = 0$ and its expansion in terms of spherical harmonics Y_{nm} in a spherical coordinate system (r,θ,φ) with its origin contained inside Ω is given by [4]:

$$\psi = \frac{1}{4\pi}\sum_{n=1}^{\infty}\sum_{m=-n}^{+n} a_{nm}\, r^n\, Y_{nm}(\theta,\varphi). \qquad (1)$$

The field is related to this potential by $\mathbf{B} = -\mu_0\nabla\psi$ and each of its components has the form

$$B_k = \sum_{n=1}^{\infty}\sum_{m=-n}^{+n} a_{nm}\; F_{k,nm}(r,\theta,\varphi), \qquad (2)$$

where the index k stands for the radial, azimuthal and polar directions of the coordinate system. The explicit forms of functions $F_{k,nm}(r,\theta,\varphi)$ are obtained by expanding the gradient operator.

The total field may be regarded as a superposition of two fields, namely the ambient field and the field generated by an external compensation system. This latter is composed by N independently fed coils. As a consequence, each expansion coefficient a_{nm} in (2) may be written in the form

$$a_{nm}(i_1, i_2, \dots, i_N) = a_{nm}^{\text{amb}} + a_{nm}^{\text{comp}}(i_1, i_2, \dots, i_N), \qquad (3)$$

where a_{nm}^{amb} and a_{nm}^{comp} stand for the expansion coefficients of the ambient and compensation fields respectively.

Equation (3) highlights that while the ambient field and its set of expansion coefficients $\{a_{nm}^{\text{amb}}\}$ are fixed, the compensation field and the coefficients in its spherical harmonics decomposition $\{a_{\text{nm}}^{\text{comp}}\}$ are functions of the coil currents i_j. Consequently, this functional dependency on the coil currents is inherited by the total field and by its own set of expansion coefficients $\{a_{\text{nm}}\}$.

A complete compensation of the ambient field would be attained everywhere in Ω if all components of the total field (2) could cancelled. In accordance with (3), such a condition would be achieved if the N currents fed to the compensation coils could be adjusted in such a way that $a_{nm}(i_1, i_2, \dots, i_N) = 0$ for all expansion coefficients in (2).

Such compensation is impossible to be performed in practice, since the ambient field cannot be generally expressed as a linear combination of the fields generated individually by a finite number of coils. On the other hand, a subset of coefficients $\mathbb{A} \subset \{a_{nm}\}$ can often be cancelled or at least minimized due to the specific design of the coil windings integrating the compensation system. This partial compensation may be quoted as a multi-objective optimization problem as follows:

$$\forall\,(a_{nm} \in \mathbb{A}) : \begin{cases} \text{minimize } f_{nm}(i_1, i_2, \dots . i_N) = (a_{nm})^2 \\ \text{subjected to } |i_j| \le I_j\,,\; j = 1,2,\dots,N \end{cases}. \qquad (4)$$

The constraints I_j above are related to the maximum permissible currents of each coil. The problem expressed by (4) can be promptly solved with the aid of standard optimization algorithms. The following remarks should be taken into account for the evaluation of objective functions f_{nm} in such a context:

- As previously mentioned, ambient field expansion coefficients a_{nm}^{amb} are fixed for a given environment. They can be identified up to any given order n by the solution of an inverse problem in accordance with (2) if a sufficient number of ambient field measurements has

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been performed in the zone of interest with the aid of well-positioned magnetometers [5].

- The functions $a_{nm}^{\text{comp}}(i_1, i_2, \dots, i_N)$ can be evaluated for any set of currents by means of an inverse problem as well. In this case a computer model of each coil is employed to generate the left-hand side of (2).

III. APPLICATION TO A FFC RELAXOMETER

The numerical scheme arising from the discussion of section II was applied to the FFC-NMR relaxometer shown in Fig. 1. Two pairs of saddle coils (S1 and S2) and the main magnet (M) of the relaxometer integrate its compensation system with the objective of cancelling the ambient field in the small volume occupied by a sample positioned inside the bore of the main magnet.

In this application, the solution of (4) is given by a triplet of current values (i_{S1}, i_{S2}, i_M) required by the aforementioned coils to create the compensation field. The spherical-harmonics decompositions required for the evaluation of the objective functions in (4) are given in Table I up to an order $n = 2$ and for three combinations of coil input currents. The spherical system of coordinates of the decompositions was fixed to the center of the magnet.

Two variants of the multi-objective optimization problem are considered, differing by two specific choices of subset $\mathbb{A}$ in (4). Each variant can be interpreted as a distinct field compensation strategy since they contemplate different field homogeneity criteria, as described in Table II.Their respective solutions are also provided in this table and were obtained with the aid of a standard genetic algorithm (500 generations, population size = 10). All three currents were subjected to constraints $|i_j| \leq 100$ mA.

IV. ANALYSIS AND CONCLUSIONS

The total field decompositions resulting after compensation are available in Table III for the two optimization objectives previously established in Table II. One may verify that the current set point given by the solution of case 1 results in an almost complete compensation of the first order decomposition coefficients of the total field. Since these coefficients are related to spatially uniform field components, this current set point could be obtained in practice by adjusting (i_{S1}, i_{S2}, i_M) by trial and error while monitoring the field inside the bore of the magnet with the aid of a magnetometer.

On the other hand, the current set point predicted by the solution of problem 2 corresponds to a non-trivial operation condition that cannot be as easily determined otherwise. Though it corresponds to a partial compensation of the second order field components, this point of operation represents the best compensation attainable for the fixed set of coils integrating the compensation system in the sense provided by (4).

The optimization approach presented in this paper may be easily extended to the compensation of fields up to any given order and for compensation systems with an arbitrary number of coils. As a consequence, the proposed optimization procedure may also be employed to design more efficient compensation systems and to give shape to very specific spatial distributions of the total field, as required by MRI applications. A detailed investigation into these features of the technique will become the object of future work.

TABLE I -. AMBIENT AND COMPENSATION FIELDS DECOMPOSITIONS

(n,m)	$a_{nm}^{\text{comp}}(1\text{mA},0,0)$	$a_{nm}^{\text{comp}}(0,1\text{mA},0)$	$a_{nm}^{\text{comp}}(0,0,1\text{mA})$	a_{nm}^{amb}
(1,-1)	3.10	2.59	0.10	-206.45
(1,0)	0.00	0.00	-28.70	-342.89
(1,+1)	2.59	-3.09	-0.01	133.31
(2,-2)	0.13	0.12	-6.93	-40.85
(2,-1)	0.00	0.00	-0.05	92.73
(2,0)	0.46	-0.51	8.56	76.10
(2,+1)	0.00	0.00	2.23	-6.16
(2,+2)	-0.26	0.29	-4.85	-22.88

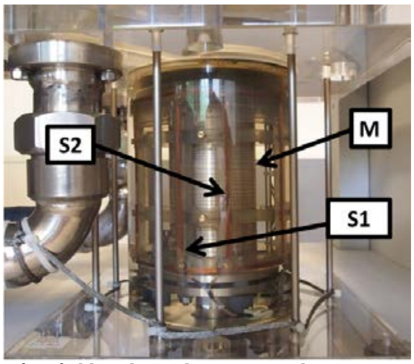

Fig. 1 – The fast-field cycling relaxometer and its compensation coils.

TABLE II - SUMMARY OF FIELD COMPENSATION PROBLEMS ANALYZED

Optimization cases	Interpretation	Solution (i_{S1}, i_{S2}, i_M) in mA
1: $\mathbb{A} = \{a_{1-1}, a_{10}, a_{1+1}\}$	Minimize uniform field components	(18.1, 58.4,-11.9)
2: $\mathbb{A} = \left\{\begin{matrix} a_{2-2}, a_{2-1}, a_{20}, \\ a_{2+1}, a_{2+2} \end{matrix}\right\}$	Minimize 1st order spatial gradient	(-50.3, -19.9, -6.4)

TABLE III – TOTAL FIELD AFTER COMPENSATION (TARGET COEFFICIENTS ARE DEPICTED IN BOLD IN EACH OPTIMIZATION CASE)

(n,m)	a_{nm} – optimization case 1	a_{nm} – optimization case 2
(1,-1)	**0.00**	-414.61
(1,0)	**-1.35**	-159.21
(1,+1)	**-0.25**	64.64
(2,-2)	51.27	**-5.59**
(2,-1)	93.38	**93.08**
(2,0)	-46.99	**8.32**
(2,+1)	-32.67	**-20.42**
(2,+2)	47.15	**15.70**

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