ARCHIVES OF ELECTRICAL ENGINEERING VOL. 60(4), pp. 433-444 (2011)

DOI 10.2478/v10171-011-0036-1

Estimation of an equivalent short solenoid model using different numerical methods*

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(Received: 07.06.2011, revised: 03.08.2011)

Abstract: This paper deals with an inverse magnetostatic problem related to the reconstruction of a permanent magnet encapsulated inside the cathode of a magnetron sputtering device. The numerical analysis is aimed to obtain the estimation of a short solenoid equivalent to the unknown magnet. Least squares approach has been used to solve the functional defined as squared sum of the residuals. A comparison of the results obtained with Genetic Algorithm approach and nonlinear system of equations is performed. A regularized solution, which is in good agreement with the experimental data, was found by applying a Newton adapted regularization technique.

Key words: solenoid model, nonlinear problem, numerical methods, least squares

1. Introduction

Magnetron sputtering devices are used for deposition of thin films, largely applicable in materials evolution. The magnetostatic configuration generated by the permanent magnets inside the cathode is a key aspect of this technique. Without detailed information of the magnetic characteristics and geometry of the permanent magnets, the determination of an equivalent model of the configuration in different conditions is not immediate. A way is to tackle the problem as an inverse one [1, 2]. In this case, it must be noted that all physical measurements are subjected to uncertainties related to the "observed value" (or a set of "observed values") and therefore electromagnetic inverse problems referring to an object or source identification by electric or magnetic field measurements, inherit also the property to be ill-posed [3].

* This is extended version of a paper which was presented at the 8th International Conference on Computation in Electromagnetics, Wrocław, 11-14.04.2011

Least squares problems are the classical approach when dealing with a parameterized application that measures the discrepancy between the model and the output of the system at various observations points. The nonlinearity of the problem is handled by utilizing different optimization algorithms like Newton-Gauss or Gradient Methods. The solution is obtained by the minimization of a functional which is defined as the norm of the discrepancy between the measured data and the calculated values for an estimated objective function. The problem of finding approximate, stable and unique solutions is referred to as regularization theory of ill-posed problems. That is, solutions of this kind of problems are non-unique and very unstable for little perturbations that occur in the process. In these cases, regularization may be used to introduce moderate assumptions on the solution and prevent overfitting. An adapted regularization formulation is applied in order to get a stable and precise solution [4].

The system under analysis is located at the Department of Electrical Engineering of the University of Padova [2].

2. Inverse identification problem

A fundamental requirement of the inverse problem is the geometrical understanding of the system. In fact, the geometry analysis reveals the most suitable strategy to provide a solution. The effective use of numerical techniques is often based on the comprehension of the main structures.

The starting model was identified from the measurements of the magnetic field components in the proximity of the cathode. Measurements of the vertical component (z axis) of stationary magnetic flux density, B, just over the cathode (Fig. 1) on the upper surface (backing plate) have been performed [2].

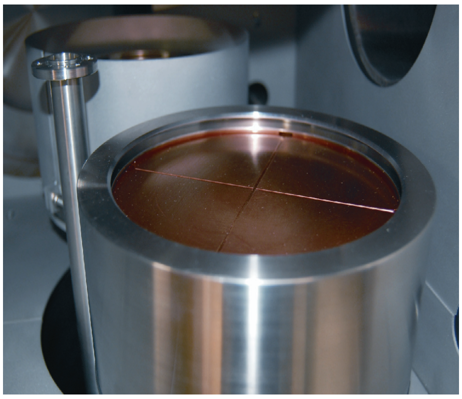

Fig. 1. The cathode under investigation

They revealed a maximum (in magnitude) at $r = 0$ and at $r = 72$ mm (Fig. 2): therefore it has been assumed that in the cathode there are: a cylindrical permanent magnet located in the center, and a coaxial cylindrical ring, with the same height, at an average radius of 72 mm.

The position $z = 0$ has been set in the barycenter of the height of the central magnet and has been experimentally identified in [2]. The assumed cylindrical permanent magnet located in the center is presented in Figure 3.

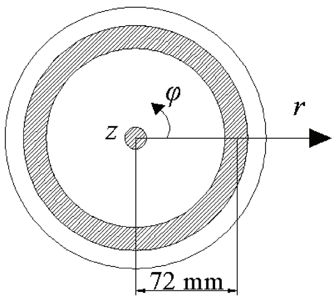

Fig. 2. Permanent magnets disposition

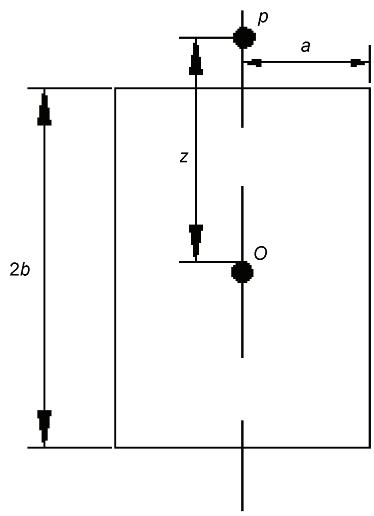

Fig. 3. The short solenoid model

Starting from the backing plate, measurements of $B_z(z)$ at different z values (from 18.5 to 24.5 mm) on the central axis have been done. These data were used for the numerical analysis of the inner magnet and are reported in Table 1.

Table 1. Experimental values of $B_z(z)$

z [mm]	18.5	19.3	20.5	21.4	22.5
B_z [mT]	311	271.9	221.9	199.7	162.9

The model of the central magnet was built, assuming that near the central axis and the central magnet, the effect of the magnetic field due to the coaxial outer ring is negligible [1, 2]. Therefore the model considers the central magnet, alone in air. The considered magnet is made of Neodymium Iron Boron (NdFeB) and is assumed with a remanence of 1.4 T.

2.1. Analytical model for the central magnet

For the central magnet, a linear B-H characteristic in the second quadrant, has been assumed according to the relation:

$$B_z(z) = B_r + \mu_0 H_z(z), \tag{1}$$

where B_r is the remanence and $\mu_0 = 4\pi*10^{-7}$ H/m. Moreover, a uniform z directed magnetization (M_z) has been taken, with $M_z = B_r/\mu_0$. Therefore, an equivalent short solenoid with circular cross-section (radius a and height $2b$), in air, has been used. The analytical formula of B_z in a stated point, related as p, (Fig. 3) on the central axis is well-known and is:

$$B_z(p) = \frac{B_r}{2}\left[\frac{z+b}{\sqrt{(z+b)^2 + a^2}} - \frac{z-b}{\sqrt{(z-b)^2 + a^2}}\right]. \tag{2}$$

3. Numerical approaches for the inverse problem

The objective of an inverse problem is to find best model, $\boldsymbol{\beta}$, such that:

$$\boldsymbol{F}(\boldsymbol{\beta}) = \boldsymbol{d}, \tag{3}$$

where $\boldsymbol{F}$ is the observation function describing the relationship between the observed data, $\boldsymbol{d}$, and the model parameters. For an inverse problem, the data are the results of some measurements, and the unknowns are the values of parameters. As indicated in the introduction, one of the difficulties arising in the solution of some problems is the instability (a small change in the inputs of the problem produces a large change in the outputs). A more essential difficulty in this type of problems is the nonuniqueness of the solution that may have multiple causes. The usual way of solving a nonlinear inverse problem is by iteration of a linearized problem. A few numerical methods with unconstrained optimization are used for solving the inverse nonlinear least squares problem [5]. The same problem is handled with Genetic Algorithm and direct implementation of nonlinear system. To reduce the instability in the recovered model parameters obtained by solving the inverse problem, a Newton Adapted regularization procedure has been applied to the nonlinear system.

The stability of the solution has been tested up to a measurement noise of 15%. First, the perturbation was applied to each measurement given in Table 1 separately and then to all at the same time. The error on the measured data was tested for both addition and subtraction and the maximum value of the change has been reported.

3.1. Least squares problem

3.1.1. The mathematical formulation of the general problem

Mathematically, the term of "least squares", is used for the problem of approximately solving an overdetermined system of equations, where the best solution is the one that minimizes the sum of squared differences between the data values and their corresponding modeled values. A nonlinear overdetermined system of equations can be written:

$$\boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{0} \tag{4}$$

with $F : R^m \to R^n$ where $m > n$. Solving a nonlinear system where multiple solutions exist is complicated and has high computational complexity. A different approach has been proposed in [6, 7].

The objective function *f*, in nonlinear least squares problems has the following form:

$$f(x, \boldsymbol{\beta}) = \frac{1}{2} \sum_{i=1}^{n} \left(y_n - f\left(x_n, \boldsymbol{\beta}\right)\right)^2, \tag{5}$$

where y_n is the observed data measured in x_n points, $\boldsymbol{\beta} = (\beta_{1,} \beta_2 \dots \beta_m)$ is the vector of the unknown parameters, and $f(x, \boldsymbol{\beta})$ represents the function model that in addition to the variable x also depends on n parameters. The errors between the measured values and the calculated values, called residuals, are given by:

$$r_i = y_i - f\left(x_i, \boldsymbol{\beta}\right), \quad i = 1 \dots n. \tag{6}$$

The aim is to find the vector $\boldsymbol{\beta}$ of parameters such that the function fits best the given data, i.e. the objective function is minimized. This occurs when the gradient of $f(x)$ is equal to zero.

The solution $\boldsymbol{\beta}$, of optimal parameters is found by solving the normal equations:

$$\left(\boldsymbol{J}^T \boldsymbol{J}\right) \boldsymbol{\beta} = \boldsymbol{J}^T \boldsymbol{y}, \tag{7}$$

where $\boldsymbol{J}$ is the Jacobian matrix and $\boldsymbol{J}^T$ is the transpose matrix of $\boldsymbol{J}$. These equations can be solved using various matrix decompositions, Newton methods or the Gradient Methods. The result is obtained iteratively, with values refined by successive approximations:

$$\beta_j^{k+1} = \beta_j^k + \Delta \beta_j, \quad j = 1 \dots m. \tag{8}$$

Because most of those algorithms proceed by minimizing the sum of squares defined above, they overlap in motivation, analysis, and implementation with optimization techniques. Features like line search and inexact solution at each iteration are important in both areas as are other issues such as derivative evaluation and global convergence. Newton method (and its derivatives) is one of the most powerful techniques in both optimization and nonlinear problems [5].

3.1.2. The nonlinear approach

The basis of the least squares when dealing with nonlinear systems of equations is to approximate the model by a linear one and to refine the parameters by successive iterations. Problems of ill-conditioning can be improved by finding initial parameter estimates that are near to the optimal values. A possible way to do this is to perform a few computer simulations, by adjusting the parameters until the agreement between observed and calculated data is reasonably good. In this case a better starting point for the nonlinear refinement was to begin from the values obtained with determined nonlinear system of equations, for which the error computed is zero. Newton-Raphson method has led to the values of: $a = 7.83$ and $b = 13.64$.

Therefore, an approximate range for the parameters was set: 6 to 9 for the radius *a,* and from a minimum value of 11 up to a maximum value of 14 mm for *b*. We considered the five data points and the corresponding experimental values of the vertical component of the magnetic flux density reported in Table 1.

The functional can be written as:

$$F = \frac{1}{2}\sum_{i=1}^{m}\left[B(z,a,b)_i - B_m(p)_i\right]^2. \tag{9}$$

Using a minimization technique, such as a gradient method the solution is found by successive iterations [5]:

$$p_{k+1} = p_k + \alpha \cdot \frac{\partial F}{\partial p}, \tag{10}$$

where $\boldsymbol{p}$ represents the unknown parameters vector and $\boldsymbol{\partial F/\partial p}$ the Jacobian matrix corresponding to the defined functional. The fastest decrease of a real-valued function *F*, that is defined and is differentiable in the neighborhood of a point *p*, is in the direction of the negative gradient of *F* at *p*, $-\boldsymbol{\Delta F}(\boldsymbol{p})$. α represents the step size which can be constant or computed within a line search procedure at each iteration. The Conjugate Gradient method proved to be very robust, the value of 8.81 found for *a,* and 12.82 for *b*, were not sensitive to the choice of the initial guess, found in the interval previously considered. The absolute error that measures how close the result is to a solution was 0.023. The same solution ($a = 8.81$ and $b = 12.82$) was found with Newton-Gauss algorithm, used in nonlinear least squares problem, to minimize the sum of squared function values. The normal equations were directly solved by applying a Cholesky decomposition to the well-conditioned full rank matrix $J(a, b)^T J(a, b)$. This method is convergent only for initial values close to the solution that is, in the range established. An example of the convergence process is shown in Figure 4.

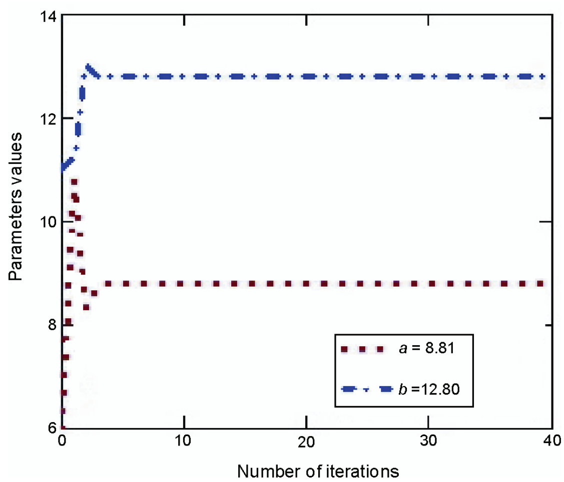

Fig. 4. Example of convergence process for Newton-Gauss method

Both methods behaved in a similar way when noises were applied to data. For Newton-Gauss method, the stability testing results are given in Table 2. A perturbation of 1% added to the first of the measurements has generated a change of approximately 2.1% in the solution; with a perturbation of 15% a discrepancy of 40.7% resulted. When the maximum value of noise (15%) was added altogether to the points the change was 29%.

Table 2. Stability testing results for Newton-Gauss method given as percentage error

Measurement [mT]	Percentage error			
	1%	5%	10%	15%
311	2.11	11.63	24.48	40.74
271	0.48	2.58	5.21	8.28
221	0.48	2.58	5.21	8.28
199	2.16	11.35	23.26	37.43
162	2.78	15.71	34.19	38.05

3.2. Genetic Algorithm

Another approach for this optimization problem was to consider the flexible systematic method of Genetic Algorithm (GA). Based on the ideas of biology, GA is a global optimization technique that performs an iterative search, starting from an initial population. It can be random or heuristically chosen.

A classical type of GA was developed in order to determine the optimal parameters, from data generated by magnetic external probing. Five measurement points of B_z, at different z heights, reported in Table 1 were imposed in equation (2), as the input data. The values, gathered from a set of 50 randomly combined pairs, with an absolute error of 0.006, were 8.45 mm for the radius a and 26.62 mm for the height $2b$ of the magnet.

The stability of GA was successfully established for linear systems in [8] and different controllers were developed for control systems [9]. The implementation of the GA for this particular case did not imply any special controller for stability. The stability testing results are reported in Table 3. Applying a perturbation of 1% to the first experimental data given in Table 1 a change of 1.08% appeared in the solution; when 15% noise was considered a change of 10.24% resulted.

Table 3. Stability testing results for Genetic Algorithm method given as percentage error

Measurement [mT]	Percentage error			
	1%	5%	10%	15%
311	1.08	7.65	9.71	10.24
271	0.92	5.61	8.65	8.28
221	0.58	5.58	7.23	6.43
199	0.64	3.12	7.1	5.78
162	0.66	4.67	6.27	7.85

Adding a 15% perturbation to all the experimental data a change of 16.1% has been noted on the solution.

3.3. Nonlinear system of equations

A solution of our identification problem is to consider the multiobjective optimization as described in [7] or to directly implement the system of nonlinear equations:

$$B(a,b)_i = B(p)_m . \tag{11}$$

The solution of (11) is found by applying a *Given-Minerr* Mathcad predefined function based on different methods. When solving with Quasi-Newton algorithm a slight variation of the solution was observed; the range of *a* started at 7.8 up to 8.5 and *b* varied from a value of 13.2 up to 13.7, for the initial guess always in the considered interval indicated in Section 3.1.2. A more robust method proved to be Levenberg-Marquardt which was not sensitive in the choice of initial values. In this case *a* equals 8.2 and *b* was 13.40. The absolute error in both cases did not exceed 0.009. The latter method was subjected to perturbation noises and the results are given in Table 4.

Table 4. Stability testing results for Levenberg-Marquardt method given as percentage error

Measurement [mT]	Percentage error			
	1%	5%	10%	15%
311	2.08	11.55	24.68	41.89
271	0.68	3.65	7.45	11.9
221	0.79	4.07	7.89	11.8
199	1.50	8.02	16.26	25.9
162	2.05	11.43	24.51	41.78

Important changes were observed when noises were added to the first value; 1% perturbation yielded to a variation of 2% of the solution and 15% perturbation gave a change of 41.89%. When noises of 15% were added to all measurements at the same time a change of 25.47% resulted.

4. Newton Adapted regularization

As it is formulated, the identification problem of the solenoid must be considered as an inverse ill-posed problem. Therefore, a regularization method has to be applied. The standard regularization for this type of problems was proposed by Tikhonov and involves minimizing the following least squares problem:

$$\min\left\{\| \boldsymbol{J}\cdot\boldsymbol{x}-\boldsymbol{y}\|^2 - \|\boldsymbol{L}\cdot\boldsymbol{x}\|^2\right\}, \tag{12}$$

where $\boldsymbol{J}$ is an ill-conditioned matrix, and $\boldsymbol{L}$ represents the penalty applied to the solution. The regularized Tikhonov solution for nonlinear problems can be found by solving the equivalent equation:

$$\left(\boldsymbol{J}^T\boldsymbol{J}+\alpha\boldsymbol{L}^T\boldsymbol{L}\right)\cdot\boldsymbol{x}=\boldsymbol{J}^T\boldsymbol{y}. \tag{13}$$

Different iterative regularization cases were studied in [10-12]. Significant results were obtained for iteratively regularized Newton-Gauss method. For the nonlinear case studied in this paper the Newton-Gauss regularization technique did not present significant stability of the solution, therefore a further improvement was added to the Tikhonov matrix, $\boldsymbol{L}$. The "Newton Adapted" algorithm given in [4] started from several initial values for the parameters, taken from the a priori given intervals.

$$p_{k+1}=p_k+\left[\left(J_k^T\cdot J_k+\alpha\cdot I\right)\cdot p_k\right]^{-1}\cdot\left[J_k^T\left(B(a,b)_k-B_m\right)+\alpha\cdot I\cdot p_k\right], \tag{14}$$

where J term is the Jacobian matrix expressed as the derivative of each parameter for every coordinate point and α represents the regularization parameter. The convergence of the process for the values of a = 8.16 and b = 13.46, for which the solution presents the smallest error, is presented in Figure 5.

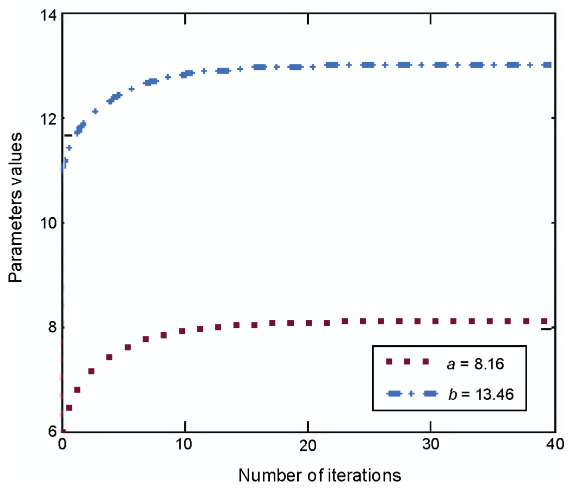

Fig. 5. Example of convergence process for Newton Adapted regularization

Satisfactory results were obtained for the cases when initial values of a and b were set in the a priori given intervals reported in Section 3.1.2. As tested for the worst cases in the aforementioned ranges, a maximum error of 9.3% was reached. If a tolerance less than 4.8% (or an absolute error of 10^{-2}) is imposed, the accepted range for each parameter resulted and they are given in Table 5. In the following analysis, the solution with the smallest error (a = 8.16, b = 13.46) has been used.

Table 5. Numerical values for a and b

a	7.74	8.04	8.16	8.34	8.65	8.95
b	13.74	13.54	13.46	13.34	13.15	12.95

It can be noticed that if the range of a and b is considered wider than the one stated in Section 3.1.2 (except when $a = b$ or when a is much smaller than b, that are cases where large errors occur), the results are still found in good agreement with the reported values, but the accuracy is significantly reduced.

The stability and the calculus error were not influenced by the choice of the regularization parameter for a value between $[10^{-5} \div 10^{-9}]$. Therefore, no special method of finding the best choice for this parameter was needed [13, 14]. The standard value was set at 10^{-7}.

As regarded the computational effort, Newton adapted algorithm was proven to be very rapidly convergent. The results are stable; which means that a small change in data implies a small change in the solution. The stability testing results are given in Table 6.

Table 6. Stability testing results for Newton Adapted regularization given as percentage error

Measurement [mT]	Percentage error			
	1%	5%	10%	15%
311	0.15	0.80	1.56	2.39
271	0.14	0.75	1.46	2.22
221	0.13	0.66	1.29	1.96
199	0.11	0.60	1.17	1.78
162	0.10	0.53	1.03	1.57

Adding a noise of 1% to the first measurement value a small change of 0.15% resulted in the solution. When the maximum perturbation is considered a value of 2.39% was recovered in the result. When 15% perturbation is added altogether to all the observed data a change of 10.09% resulted.

5. Results

In order to quantify the above discussed methods, the values of B_z, measured on the central axis, on five points have been taken as reference for the comparison. Equation 2 has been used, with a and b values obtained with the numerical methods. The results are reported in Table 7.

Table 7. $B_z(z)$ values on the central axis: experimental data and values obtained by combining equation (2) with the numerical output

z [mm]	Measure [mT]	Newton-Gauss [mT]	Genetic Algorithm [mT]	Given-Minerr Levenberg-Marquardt [mT]	Newton Adapted [mT]
18.5	311	295	310	308	310
19.3	271.9	260	273	270	272
20.5	221.9	217	225	222	223
21.4	199.7	190	196	193	193
22.5	162.9	162	166	162	163
23.4	147.2	142	145	142	142
24.5	121.8	122	125	121	121

Genetic Algorithm and Levenberg-Marquardt methods fit the experimental data with an error close to 4.8%. Highest error (8.9%) between the measurements and the numerical results was found for the method of Newton-Gauss. Best fit (4.4%) was obtained with Newton-Adapted regularization. Stability to perturbations has been performed and the results are presented in Tables 3-5 respectively. The percentage error is higher when the noise is applied to the first value and it can be seen that the regularization technique in terms of Newton Adapted method proved to be effective for both stability and precision.

6. Conclusions

An inverse problem of short solenoid model identification by magnetic flux density measurements was proposed. The problem proves to be ill posed and thus with an unstable solution. Several methods of finding the problem parameters were detailed. The most satisfying behaviour with respect to stability and accuracy was achieved with the Newton Adapted regularization technique.

Acknowledgment

This paper was supported by the project *Doctoral studies in engineering sciences for developing the knowledge based society-SIDOC* contract no.POSDRU/88/1.5/S/60078, project co-funded from European Social Fund through Sectorial Operational Program Human Resources 2007-2013 and TE_253 Project.

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