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Computer-aided design of a dielectric insert supporting uniformity of fast microwave heating

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Abstract

Purpose – This paper aims to introduce and illustrate a computational technique capable of determining the geometry and complex permittivity of a supplementary dielectric insert making distributions of microwave-induced dissipated power within the processed material as uniform as possible.

Design/methodology/approach – The proposed technique is based on a 3D electromagnetic model of the cavity containing both the processed material and the insert. Optimization problem is formulated for design variables (geometrical and material parameters of the insert) identified from computational tests and an objective function (the relative standard deviation [RSD]) introduced as a metric of the field uniformity. Numerical inversion is performed with the method of sequential quadratic programming.

Findings – Functionality of the procedure is illustrated by synthesis of a dielectric insert in an applicator for microwave fixation. Optimization is completed for four design variables (two geometrical parameters, dielectric constant and the loss factor of the insert) with 1,000 points in the database. The best three optimal solutions provide RSD approximately 20 per cent, whereas for the patterns corresponding to all 1,000 non-optimized (randomly chosen) sets of design variables this metric is in the interval from 27 to 136 per cent with the average of 78 per cent.

Research limitations/implications – As microwave thermal processing is intrinsically inhomogeneous and the heating time is not a part of the underlying model, the procedure is able to lead only to a certain degree of closeness to uniformity and is intended for applications with high heating rates. The initial phase of computational identification of design variables and their bounds is therefore very important and may pre-condition the "quality" of the optimal solution. The technique may work more efficiently in combination with advanced optimization techniques dealing with "smart" (rather than random) generation of the data; for the use with more general microwave heating processes characterized by lower heating rates, the technique has to use the metric of non-uniformity involving temperature and heating time.

Practical implications – While the procedure can be used for computer-aided design (CAD) of microwave applicators, a related practical limitation may emerge from the fact that the material with particular complex permittivity (determined in the course of optimization) may not exist. In such cases, the procedure can be rerun for the constant values of material parameters of the available medium mostly close to the optimal ones to tune geometrical parameters of the insert. Special manufacturing techniques capable of producing a material with required complex permittivity also may be a practical option here.

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Originality/value – Non-uniformity of microwave heating remains a key challenge in the design of many practical applicators. This paper suggests a concept of a practical CAD and outlines corresponding computational procedure that could be used for designing a range of applied systems with high heating rates.

Keywords Optimization, Electromagnetic fields, Modelling, Dielectric properties, Energy dissipation

Paper type Research paper

1. Introduction

While microwave heating is known for its ability to improve the efficiency and quality of a variety of applied thermal processes, the intrinsic non-uniformity of microwave-induced temperature fields remains a central challenge in designing many practical applicators. Numerous techniques aiming to homogenize temperature distribution have been reported, (Heeren and Baird, 1971; Kashyap and Wyslouzil, 1977; Bernhard and Joines, 1996; Chan and Reader, 1996; Bradshaw *et al.*, 1997; Wäppling-Raaholt and Ohlsson, 2000; Dincov *et al.*, 2004; Domínguez-Tortajada *et al.*, 2005; Wäppling-Raaholt and Ohlsson, 2005; Wäppling-Raaholt *et al.*, 2006; Cordes and Yakovlev, 2007; Domínguez-Tortajada *et al.*, 2007; Geedipalli *et al.*, 2007; Pedreño-Molina *et al.*, 2007; Basak and Badri, 2011; Koskiniemi *et al.*, 2011; Liao *et al.*, 2016; Wäppling-Raaholt *et al.*, 2016). It has also been shown (Lurie and Yakovlev, 2002) that the method of optimal material design can be used to determine the position and micro-geometry of composite dielectric layers that bring the electric field of the dominant mode within a rectangular dielectric prizm closest to uniformity. However, all these approaches appear to apply only in particular circumstances and/or to particular apparatuses, so new techniques suggesting both conceptual options and specific mechanisms of control of distribution of heating patterns are still on demand.

In this paper, going beyond the principles of the approach in Lurie and Yakovlev's (2002) study, we introduce a technique for determining the geometry and complex permittivity of a supplementary homogeneous dielectric insert making distribution of microwave-induced dissipated power in the given processed material as uniform as possible. As such, the proposed technique may be used for homogenizing temperature fields in a wide range of applicators designed for fast microwave heating, i.e. for the thermal processes in which the rate of heat diffusion because of thermal conductivity is lower than the rate of dissipation of electromagnetic power. The technique is based on full-wave computational analysis of the scenario and identification of geometrical parameters of the insert that are suitable for being design variables of an optimization problem. Complex permittivity of the insert is also included in the set of design variables. An objective function is linked with a characteristic of uniformity of the pattern of dissipated power. By solving the optimization problem, we determine geometrical and material parameters of the insert that make the distribution of dissipated power most uniform.

We demonstrate functionality of our technique by describing an illustrative computer-aided design (CAD) of a supplementary dielectric block in an applicator based on a rectangular waveguide and intended to be used in a particular implementation of the technology of microwave fixation (Modak *et al.*, 1976). The geometry and complex permittivity of the insert are determined for the processed material of a conical shape and dielectric properties of brain. It is shown that, in contrast to the case of non-optimized (random) parameters, the insert with optimized characteristics substantially improves the level of uniformity of patterns of dissipated power. We also discuss the ways of making the proposed technique computationally more practical, more efficient and applicable to a wider class of microwave applicators.

2. Technique

The concept of the proposed technique of homogenization of a microwave heating pattern can be outlined (with the help of Figure 1) as follows. We assume that the process takes place in a closed cavity, and frequency of excitation is constant. In an empty cavity [Step (A)], an adopted excitation generates the time-maximum field pattern $\mathbf{E}_0$. When the processed material (P) is placed inside the cavity [Step (B)], $\mathbf{E}_0$ is disturbed, and the new field, called $\mathbf{E}_1$, induces a (generally, non-uniform) distribution of dissipated power $\mathbf{P}_{d1}$ within P (and thus makes it non-uniformly heated). With a supplementary dielectric insert (I) placed in the cavity [Step (C)], the field is again modified; here, we denote the new electric field by $\mathbf{E}_2$ and corresponding dissipated power by $\mathbf{P}_{d2}$. In this context, one can think of finding the geometry and material properties of I that would make $\mathbf{P}_{d2}$ as close to uniform as possible.

This problem can be solved with the help of a computational procedure based on a full-wave 3D model of the cavity filled with P and I. At the first stage, the model is used to identify, through a series of simulations, geometrical parameters g_1, [. . .], g_n of scenario (C) that, when varying, make a most notable impact on $\mathbf{P}_{d2}$. Distribution of dissipated power may also strongly depend on the dielectric constant $\varepsilon'_{\mathrm{I}}$ and the loss factor $\varepsilon''_{\mathrm{I}}$ of the insert. All these characteristics $\{g_1$, [. . .], g_n, $\varepsilon'_{\mathrm{I}}$, $\varepsilon''_{\mathrm{I}}\}$ constitute a set of design variables in an optimization problem with the goal of minimizing divergence of $\mathbf{P}_{d2}$ from uniformity and the level of homogeneity of dissipated power defined through an appropriate metric. The optimization problem is numerically solved by processing the data correlating the design variables as input parameters of the model and the pattern of dissipated power as its output characteristic. Appropriate numerical inversion leading from the most uniform $\mathbf{P}_{d2}$ to corresponding values of the design variables answers the question about the geometrical and material parameters of the insert that best homogenizes the heating pattern.

3. Computational procedure

The described computational procedure is based on a fully parameterized, 3D conformal finite-difference time-domain (FDTD) model of scenario (C). The model is run multiple times to generate a database including the design variables as input data and corresponding patterns of dissipated power as output results. In the optimization problem, the upper and lower bounds of the insert's geometrical parameters $g_1, \ldots, g_n$ are set in accordance with limitations dictated by system's practical design. In general, a wide range of possible values of $\varepsilon'_{\mathrm{I}}$ may be beneficial as allowing for a wider variety of corresponding patterns of dissipated power. On the other hand, it may be feasible to set an upper bound for $\varepsilon''_{\mathrm{I}}$ on a relatively low level and thus avoid energy-inefficient optimal designs in which the insert would be excessively heated itself.

To characterize the level of uniformity of dissipated power within the processed material, an appropriate metric needs to be defined. While several approaches were suggested for assessing the uniformity of microwave-induced temperature field (Wäppling-Raaholt and Ohlsson, 2005; Geedipalli *et al.*, 2007; Cordes and Yakovlev, 2007), there still seems to be no commonly accepted criterion. For the purposes of this work, we introduce, following Wang *et al.* (2005), Chen *et al.* (2017), Bedane *et al.* (2017), Ozturk *et al.* (2017) and Ozturk *et al.* (2018), a simple metric based on the relative standard deviation (RSD) of the values of dissipated power in the FDTD cells within the processed material:

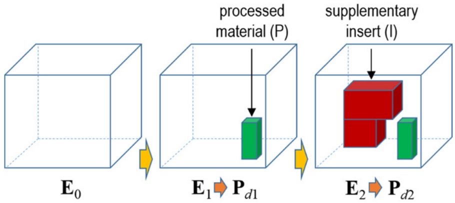

Figure 1.
Transformation of the electric field and corresponding patterns of dissipated power

$$RSD[\%] = (STD/AVG)100, \tag{1}$$

where STD and AVG are the standard deviation and the mean of the values in the pattern, respectively. Low RSD indicates that the data set has little variation, and that means that the pattern of dissipated power is relatively uniform; large values of RSD (including those over 100 per cent) represent highly non-uniform distributions.

The key steps of the procedure are outlined in Figure 2. It starts from systematic computations of patterns of dissipated power for different geometrical and material parameters of the insert and identification of those, which are most effective in terms of changing the field structure (and thus most suitable for being N design variables of the system). At Step 2, a comprehensive database containing M_0 points is generated from randomly chosen vectors:

$$\mathbf{x} = \{g_1, \ldots, g_n, \varepsilon'_{\mathrm{I}}, \varepsilon''_{\mathrm{I}}\}^T \tag{2}$$

taken from within the design space and corresponding FDTD solutions (i.e. patterns $\mathbf{P}_{d2}$), M_1 points corresponding to highest levels of uniformity are chosen. At Step 3, a sensitivity analysis is performed with the M_1 points; this is done by variation over the different components of the vector, while all others are kept constant. The purpose of this analysis is to reduce the number of design variables (down to L) and the intervals of their variation. At Step 4, optimization is performed using L design variables with the bounds of variations redefined at Step 3.

A constrained optimization problem is formulated as:

$$\min_x RSD(\mathbf{x}) \text{subject to } \mathbf{l}_b \le \mathbf{x} \le \mathbf{u}_b, \tag{3}$$

where $\mathbf{l}_b$ and $\mathbf{u}_b$ are the vectors of lower and upper bounds, respectively, for the design variables $\mathbf{x}$. Problem (3) involves only numerical data, and this issue can be handled through the use of the method of sequential quadratic programming (SQP) which does not require an analytical expression of the objective function. The problems are solved through formulation of a QP sub-problem based on a quadratic approximation of the Lagrangian function, and the Hessian is approximated with each new solution using a quasi-Newton method. Once the QP problem is solved, the solution represents the direction to be used in a standard search

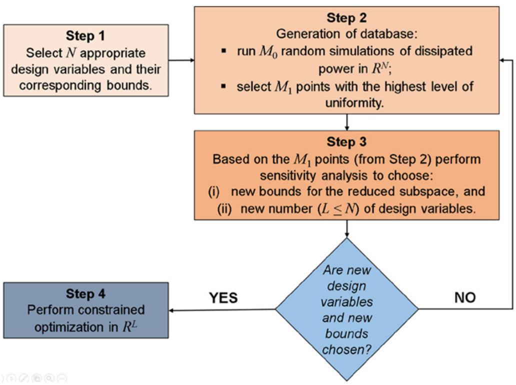

Figure 2.
Flow-chart of the computational procedure

procedure to determine the length of the step. The determined incumbent solution is used to approximate the next Hessian. This constrained optimization problem at Step 4 is solved with fmincon function in the MATLAB Optimization Toolbox (MATLAB, 1984-2017).

The described computational procedure was implemented in a dedicated MATLAB code controlling optimization via fmincon and underlying FDTD simulations performed by QuickWave (QWED, 1998-2017).

4. Example – applicator for microwave fixation

Functionality of the developed technique is illustrated by synthesis of a supplementary insert I in a 2.45 GHz applicator for microwave fixation. Microwave fixation is the technology used in post-sacrifice chemical analysis of brain chemistry. While keeping it constant after death through freezing was the primary method of studying brain chemistry on animals, rapid microwave heating has emerged as a chemically feasible and promising alternative (Modak *et al.*, 1976). Designing efficient systems capable of rigid control over this process is a difficult task as microwave thermal processing is intrinsically non-homogeneous, whereas the apparatuses for microwave fixation must provide the required level of temperature uniformity (80-90°C) precisely in the brain tissue. Appropriate CAD appears to be necessary to ensure the development of an efficient microwave system for this application.

The considered applicator (Figures 3-4) (Moon *et al.*, 2015) consists of a section of a single-mode rectangular waveguide (cross-section $a \times b$, length w), centrally connected with a cylindrical cavity of diameter C and length R such that $C > a$. The processed material (P) has a form mimicking a shape of a mouse: a body (a cylinder of diameter B and length l_3 plus a truncated cone of length l_2) and a head (a truncated cone with diameter of the base

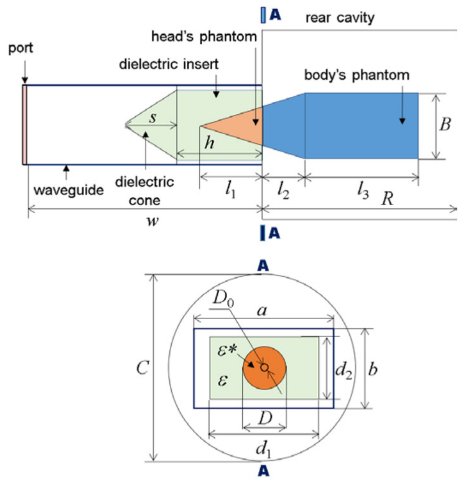

Figure 3.
Sketch of the considered system for microwave fixation (Moon *et al.*, 2015)

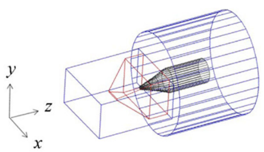

Figure 4.
3D view of the microwave system in Figure 3

D, diameter on the top D_0, and length l_1). The latter part is a volume of interest: this is where the heat release is expected to be uniform. This part of P is surrounded by the insert I: it has a shape of a rectangular block (cross-section $d_1 \times d_2$, length h) supplemented on the side facing the input of the applicator, by a pyramidal element aiming to improve matching of the loaded system with the microwave generator. This insert is expected to notably improve uniformity of heat release in its internal space filled with the truncated cone imitating the mouse's head.

Below we present the optimal geometrical and material parameters of the insert that were obtained for $a \times b = 86 \times 43$ mm (WR340), $h = 30$ mm, $D = 20$ mm, $D_0 = 5$ mm, $l_1 = 25$ mm, $w = 120$ mm, $C = 150$ mm, $R = 130$ mm, $B = 35$ mm, $l_3 = 60$ mm and $l_2 = 20$ mm. Complex permittivities of the body's and head's phantoms were taken to be the same and equal to $\varepsilon = 46.9 - j7.2$; this value is typical for a mouse brain (gray tissue) (Burdette *et al.*, 1980).

In Step 1, we identify four parameters associated with the dielectric insert, ε'_I, ε''_I (represented by electric conductivity σ), d_1 and d_2, as design variables ($N = 4$). As d_1 and d_2 are conditioned by the physical dimensions of the applicator, corresponding intervals for those parameters are chosen as:

$$30 \leq d_1(\text{mm}) \leq 80;\ 50 \leq d_2(\text{mm}) \leq 60. \tag{4}$$

However, observing from the computational experiments, a mild effect of parameter d_2 on the distribution of dissipated power and aiming to simplify the illustrative optimization, we set it constant in the middle of the interval at 55 mm. This means that, in the considered illustration, we are in a position to reduce the number of design variables (from $N = 4$ to $L = 3$) at Step 1 rather than at Step 3 when performing sensitivity analysis of *RSD*.) Next, assuming that possible variations of both dielectric constant and the loss factor can take place in very wide ranges, we set up the intervals of variation of ε' and σ in accordance with the four zones in the complex permittivity plane that are shown in Figure 5:

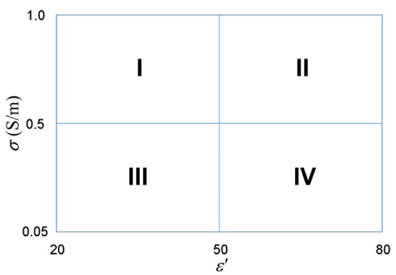

Figure 5.
Four zones of variation of ε' and σ

Table I.
Output of Step 1: values of three design variables (with $d_2 = 55$ mm) for four lowest *RSD*

Zone and point #	IV: 782	IV: 830	IV: 630	III: 185
ε'	51.0	52.6	60.6	37.9
σ (S/m)	0.202	0.333	0.308	0.274
d_1 (mm)	59.0	57.0	54.8	62.4
RSD (%)	20.75	21.40	22.98	29.10

$$\begin{array}{l}\text{Zone I}: 20 \le \varepsilon_I' \le 50;\ 0.5 \le \sigma(\mathrm{S/m}) \le 1.0;\\ \text{Zone II}: 50 \le \varepsilon_I' \le 80;\ 0.5 \le \sigma(\mathrm{S/m}) \le 1.0;\\ \text{Zone III}: 20 \le \varepsilon_I' \le 50;\ 0.05 \le \sigma(\mathrm{S/m}) \le 0.5;\\ \text{Zone IV}: 50 \le \varepsilon_I' \le 80;\ 0.05 \le \sigma(\mathrm{S/m}) \le 0.5.\end{array} \text{ and} \tag{5}$$

With design variables chosen and sub-spaces identified, we move onto Step 2 in the procedure and generate M_0 = 1,000 points of the database; without knowing its necessary size, the value of M_0 is chosen as an arbitrary large number. Random values are chosen within the interval in Problem (4) for d_1 and both intervals in a particular Zone in Problem (5). It turns out that the design variables resulting in low levels of *RSD* are obtained only for Zones III and IV: there are 2 and 22 points, respectively, corresponding to the condition *RSD* < 30 per cent.

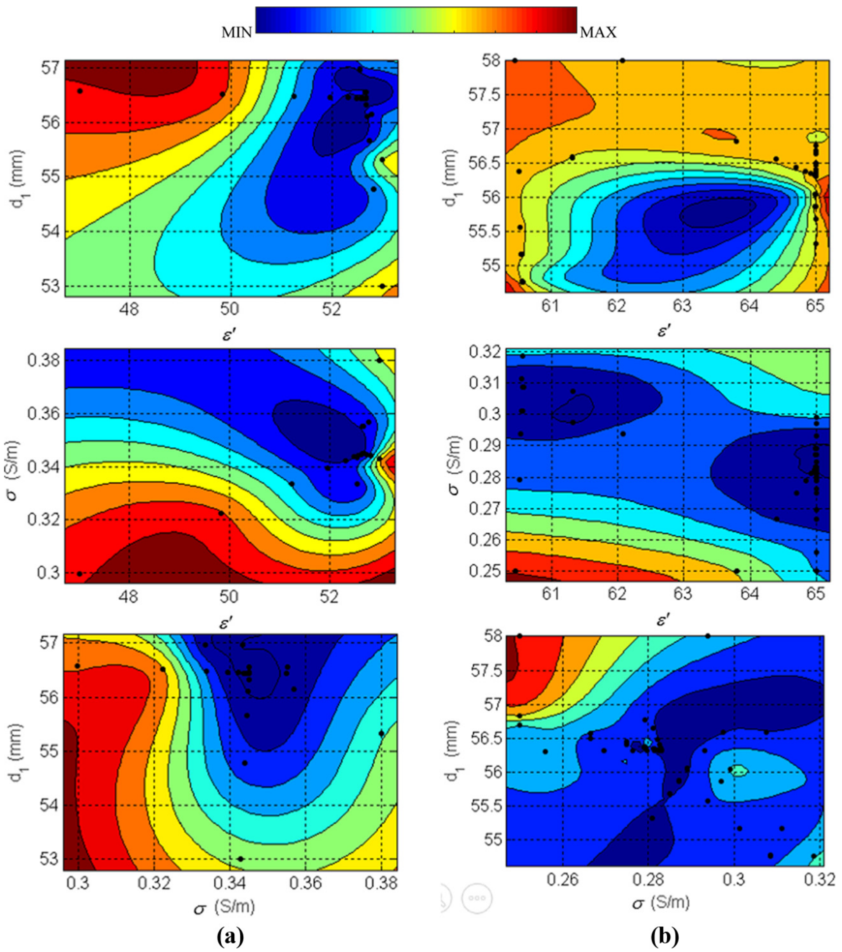

Figure 6.
Performance of the SQP optimization in the sub-spaces of three design variables (d_1, ε_I' and σ) starting from points IV: 830 (a) and IV: 633 (b)

We then pick up four sets of the design variables corresponding to the lowest values of *RSD* (and highest levels of uniformity), with three coming from Zone IV and one from Zone III (so that $M_1 = 4$); those values are presented in Table I. A series of simulations performed around these points reveal that they indeed represent local minima. The sensitivity analysis also shows that d_2 is not of much influence on the value of *RSD*. Thus, at Step 3, we confirm a feasibility of reducing the number of design variables down to $L = 3$.

At Step 4, we seek better solutions for local minima. The paths the optimization technique goes along when looking for them are illustrated in Figure 6 for two points in Zone IV. The graphs show level curves in two-dimensional domains around those points, and black dots depict the points at which the optimization procedure stopped before reaching a minimum. The optimized solutions are shown in Table II. Corresponding patterns of dissipated power are characterized by *RSD* equal to 19.1, 19.3, 20.5 and 27.5 per cent; these are visualized in Figure 7 – one can see there the distributions which are quite uniform within the region of interest. For comparison: the values of *RSD* for $M_0 = 1{,}000$ set of non-optimized (randomly chosen) design variables vary from 27 to 136 per cent with the average of 78 per cent, whereas in the absence of the insert it is equal to 111.5 per cent.

5. Discussion and conclusion

We have introduced a CAD technique capable of finding the geometry and material properties of a supplementary dielectric insert which, when placed inside a microwave applicator, homogenizes distributions of dissipated power within the processed material. The approach is based on an electromagnetic model and therefore does not deal with microwave heating time. As such, the proposed technique can be used as a part of engineering system design for applicators with high rates of microwave thermal processing. An illustrative example of application of this technique to the system for microwave fixation shows operational functionality of the computational procedure and details of its possible implementation.

The phase of identification of design variables and their bounds appears to be critical for eventual success (in terms of *RSD* values) at the optimization stage. As the distribution of

Minimum near the point #	IV: 782	IV: 830	IV: 633	III: 185
ε'	50.9	52.7	65.0	38.5
σ (S/m)	0.198	0.345	0.283	0.276
d_1 (mm)	59.0	56.4	56.3	61.8
RSD (%)	20.48	19.09	19.34	27.51

Table II. Output of step 4: optimized design variables (with *d2* = 55 mm) and corresponding *RSD*

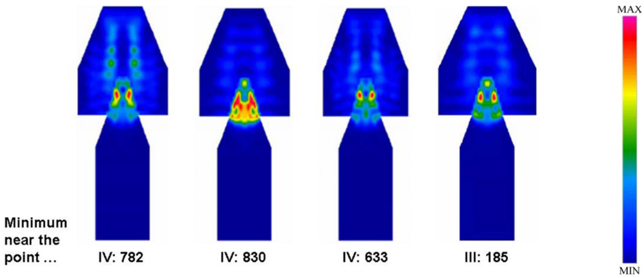

Figure 7. Patterns of dissipated power corresponding to the optimized design variables in Table II

dissipated power in an applicator is predetermined by its geometrical characteristics and materials parameters, some design sub-spaces can contain local optima of better or worse "quality" than the others. In this sense, solution of the optimization Problem (3) in this paper is expected to be particularly beneficial when the technique is applied in combination with modeling focused on finding a most promising space of design variables. This also justifies the use in the considered illustration of massive random search for the vicinities of "good" solutions at Step 2 and wide ranges for the design variables.

The proposed technique can be implemented with the use of alternative components. The RSD used in this paper as a simple metric of the level of non-uniformity of patterns of dissipated power can be replaced by a suitable goal function adequately characterizing the desirable field distribution. One can use an advanced optimization method (e.g. based on machine learning or genetic algorithms, artificial neural networks, etc.) that would deal with "smart" (rather than random) generation of the data, or a 3D electromagnetic model based on another numerical technique (e.g. finite element method) and so on. To be applied to more general (slower) microwave heating processes, i.e. those in which thermal diffusion (because of thermal conductivity) cannot be overlooked, the technique should work with the metric of uniformity formulated for the patterns of temperature field. The latter could be produced by one of the appropriate electromagnetic-thermal coupled models [reviewed by Koutchma and Yakovlev (2010)], and the metric should have microwave heating time involved in the consideration.

Multiple local solutions of the optimization problem may be a convenient option in practical design. For example, if an optimum is characterized by high value of the loss factor ε''_I that may result in an undesirable degree of heating of the insert, it may be possible to pick up another optimal solution with a lower value of ε''_I. On the other hand, in applications and adaptations of our technique to other scenarios, normalization of numerical ranges of the design variables (e.g. to the 0 to 1 interval) may be beneficial in handling redundancy.

A particular issue associated with application of the described technique comes from the fact that the material to be used in the synthesized insert should have a particular complex permittivity, which may not be available among the existing/accessible substances. In this case, the procedure can be applied again for the constant values of ε'_I and ε''_I of the available material mostly close to the optimal one to tune geometrical parameters of the insert. Also, a special technique capable of producing a material with desired dielectric constant and the loss factor (Yeung and Yakovlev, 2016; Vaucher *et al.*, 2017) appears to be (at least for low values of complex permittivity) a promising practical option. On the other hand, in some applications, satisfactory solution could be obtained from the optimization problem formulated only for geometrical parameters of the insert, i.e. without including ε'_I and ε''_I in the design variables.

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