RBF NETWORK OPTIMIZATION WITH CORS SAMPLING FOR PRACTICAL CAD OF MICROWAVE APPLICATORS

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This paper is concerned with application of an advanced neural network optimization technique to the microwave applicators in order to improve their energy coupling. The optimization algorithm features an objective function measuring the bandwidth of the frequency characteristic of the reflection coefficient over a specified optimality zone and constrained optimization response surface (CORS) technique selecting additional sample points in the dynamic training of the RBF network. The algorithm backed by 3D FDTD data is capable of exceptionally quick convergence to the optima due to a dramatically reduced number of underlying full-wave analyses. This makes this optimization technique applicable to applied electrically large systems of microwave power engineering. Functionality of the algorithm is illustrated by two examples: designing a microwave oven with a load on a glass shelf and scaling-up a reactor for microwave-assisted organic synthesis. It is shown that the optimal designs of these systems are found from 5- and 7-parameter optimizations while requiring only a few dozen/hundred simulations.

Introduction

Despite the present significant interest in optimization and computer-aided design (CAD) of systems of microwave power engineering, computational resources available for efficient virtual prototyping of practical applicators still can be considered somewhat limited. Optimization techniques based on the full-wave electromagnetic simulations appear to be attractive for complex microwave systems. However, their direct CAD may require a large number of design variables to be involved, and hence, even with not too high computational cost of direct simulation, be not viable.

Applicability of simulation-backed optimization procedures to practical systems can be improved by (*i*) increased computer productivity, and (*ii*) a reduced number of full-wave analyses. The hardware-based developments in the first direction give the modelers an opportunity to remove the 3 GB RAM limit in 64-bit operating systems and to leverage the massive parallel processing capabilities using the GPU technology [1]. The issue of reducing the number of FDTD simulations has been explicitly addressed in our earlier paper [2]. The method proposed there consists of an FDTD-backed artificial neural network (ANN) algorithm featuring special mechanisms directly responsible for the ability of the technique to find a "good" local optimum in specified domains with the use of relatively small data sets. Those mechanisms include the decomposed radial basis function (RBF) network, its dynamic training which adds specially chosen point(s) at each iteration, an objective function (OF) that accurately represents the goal of the problem, and some other features.

Furthermore, in [4], we have introduced the upgrade of the technique [2] that dramatically outperforms its predecessor due to using constrained optimization response surfaces (CORS) sampling [3] and a more accurate OF. This new one measures the bandwidth of the frequency response of an *S*-parameter over specified optimality zones. This is found to more accurately represent the goal of finding an optimal design corresponding to the characteristic below/above a given tolerance.

In this paper, we apply the optimization algorithm [4] to the electrically large applicators to show a capability of this technique to do a substantially better job in increasing energy efficiency of microwave heating systems [5]. After a brief introduction of the algorithm, we describe its performance in two applied CAD scenarios – about a microwave oven with a load on a shelf and a microwave chemistry reactor. We show that with the use of the technique [4] optimization of complex microwave applicators with 5 and 7 design variables may require as little as a few dozen or hundred analyses.

Optimization Technique: RBF Network and Objective Functions

In accordance with [4], the decomposed RBF ANN shown in Fig. 1 and denoted as $F: X \rightarrow Y$ works with input vectors $X_i = [x_1\ x_2\ \ldots\ x_N]$, where $x_1, \ldots, x_N$ are design variables for $i = 1, \ldots, P$, and P is the number of input-output pairs of modeling data. The network output vectors are obtained by taking frequency characteristics of an *S*-parameter over specified frequency range(s) given by the formula

$$Y_i = \max_{1 \le j \le n}\{[BW(S(f_j^1 \le f \le f_j^2, X_i), T_j) + 1]^{-1}\} \qquad (1)$$

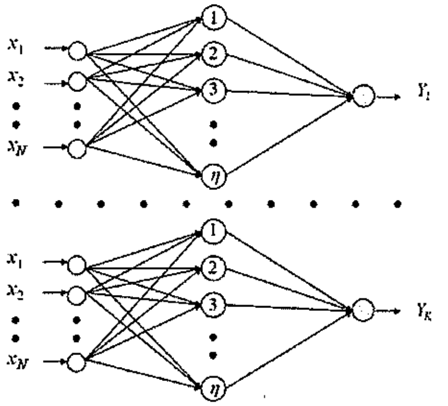

Fig. 1. Architecture of a decomposed RBF ANN with η hidden neuron.

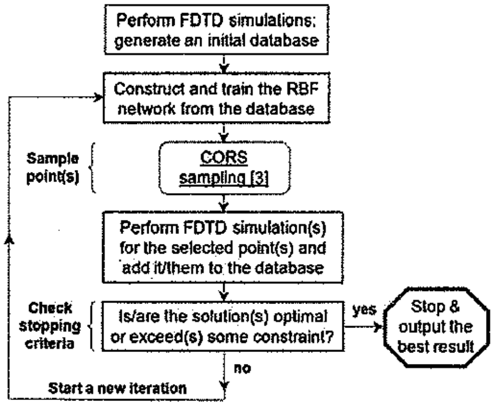

Fig. 2. Flow chart of the RBF optimization algorithm with CORS sampling.

where BW (the bandwidth) is calculated over the specified frequency interval(s) and is in the range [0, 1]. This OF represents a typical practical need of microwave optimization to search not just the minimum of S, but rather the maximum BW in a certain frequency range. The RBF used in the network is a thin plate spline defined as

$$\varphi_l^{(i)} = \begin{cases} \| X_i - c_l \|_2^2 \log(\| X_i - c_l \|_2), & \| X_i - c_l \|_2 > 0, \\ 0, & \| X_i - c_l \|_2 = 0, \end{cases} \tag{2}$$

where $l = 1, \ldots, N_c$, N_c is the number of RBFs, c_l are the centers of $\varphi_l^{(i)}$. Similarly to [2], the training set is the set of centers chosen. The network is coupled with a linear model, and the weights are constructed by solving the corresponding linear system.

A flow chart of the algorithm is given in Fig. 2. Given some initial data, we construct and train the RBF network $F(X)$, perform CORS sampling [3], simulate the sampled point, check stopping criteria, and repeat the cycle, if necessary. The most critical part of the algorithm is the choice of the sampled point. With CORS sampling, it balances the goal of finding the minimum with exploring unknown regions of the domain. This is accomplished by selecting a parameter β ($0 \leq \beta \leq 1$) and finding the minimum of $F(X)$, subject to $\|X - X_j\| \geq \beta\Delta$ for $1 \leq j \leq P$, where $\Delta = \max_X(\min_{1 \leq j \leq P} \|X - X_j\|)$.

The algorithm is implemented as a MATLAB code. Data for the network are generated by *QuickWave-3D* [6]. All CPU times are given for a Xeon 3.2-GHz PC operating under Windows XP.

Illustrative Results

In this section, functionality of the optimization algorithm is illustrated by two examples considered as open-ended practical CAD problems of microwave power engineering

Microwave Oven. In the first illustration, we find optimal configuration of a microwave oven containing a glass shelf, a cylindrical sample of processed material on it and an exciting waveguide (Fig. 3). Given the sample's diameter D, height H, and material parameters varying with temperature, we find (a) the dimensions of the shelf (d and t), (b) its position above the bottom (h), and (c) the position of the load (d_x and d_y) such that the reflection coefficient of the system ($|S_{11}|$) does not exceed 0.3 (i.e., less than 9% of microwave energy is reflected) in 75% of the frequency range from 2.4 to 2.5 GHz.

In accordance with this goal, the parameters chosen constant in this optimization problem are A = 290 mm, B = 300 mm, C = 185 mm, g_a = 86 mm, g_b = 43 mm, s = 10 mm, D = 60 mm, H = 70 mm, and $\varepsilon_1 = 6.0 - j0$, whereas the load's material is taken to be the resin R498 with dielectric constant and electric conductivity specified in Table 1. The five design variables are allowed to be in the intervals:

$$4 \leq t \leq 16 \text{ mm},\ 15 \leq h \leq 35 \text{ mm},\ 220 \leq d \leq 270 \text{ mm},\ -50 \leq d_x \leq 50 \text{ mm},\ 0 \leq d_y \leq 60 \text{ mm} \tag{3}$$

The procedure starts with an initial database (DB) of 100 randomly chosen points in the specified domain. The underlying FDTD model consists of 166,000 to 196,000 cells of 8 mm in air and 4.5 mm in the load, and one analysis of the system involves 20,000 time-steps (2.2 to 2.6 min of CPU time).

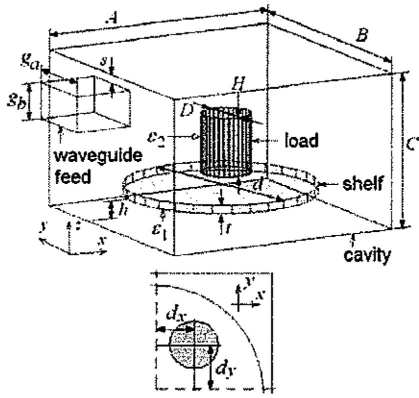

Fig. 3. Schematic view and geometrical parameters of the microwave oven.

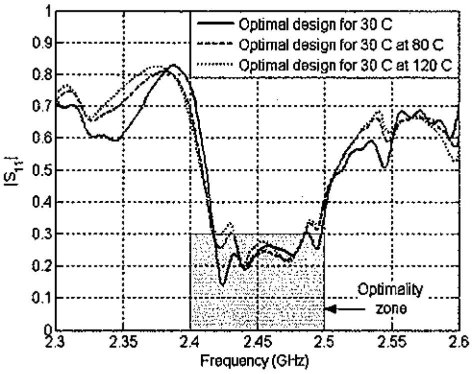

Fig. 4. Reflection coefficient $|S_{11}|$ in the optimized microwave oven with the processed material at its initial (30°C) and high (80 and 120°C) temperatures.

Table 1. Material Parameters of Resin R498 as Measured in [7]

Temperature, °C	Dielectric constant, ε'	Electric conductivity, σ (S/m)
30	5.05	0.240
80	6.91	0.375
120	7.79	0.283

Table 2. Microwave Oven: Optimized Configurations for Different Temperatures of R498

Temperature, C	t	h	D	d_x	d_y	No of FDTD analyses
30	16.0	35.0	230.3	46.6	0	177
80	16.0	35.0	232.1	43.7	11.4	704
120	16.0	31.8	220.0	45.0	14.1	315

When optimizing this oven, the RBF CORS technique achieves the objective with different number of FDTD analyses including the case of very quick convergence to the optimal solution for 30°C; the values of the optimized design variables are collected in Table 2. The $|S_{11}|$ curve corresponding to the geometry optimized for the initial temperature is shown in Fig. 4 along with the graphs characterizing this system with the material at 80 and 120°C. It is seen that this optimal configuration may not provide the same level of performance at higher temperatures – the bandwidth of the system deteriorates to ~55%. Similar analysis for 80 and 120°C shows the reduction in *BW* down to ~57 and ~34% respectively leaving to the designer the choice between the first and the second geometries.

Microwave Chemistry Reactor. Here we consider a conventional reactor for microwave-assist organic synthesis (Fig. 5). The cavity contains a thin-wall vessel with a reactant whose volume V is assumed to be fixed. The reactor is excited by a rectangular waveguide which may be offset in the x- and y-directions by f_x *and* f_y respectively. The vessel also may be offset from the center by v_x *and* v_y being located a distance s from the top of the cavity. The optimization problem is: given the height H and the processed reactant, find the configuration of the whole system, i.e., diameter D, dimensions of the reactant (d and h), its position in the cavity (s, v_x and v_y), and a position of the waveguide, that yields less than 1% of reflected microwave energy (i.e., $|S_{11}| < 0.1$) in the frequency range 2.4 to 2.5 GHz.

In accordance with this goal, the parameters chosen constant in this optimization are $H = 300$ mm and $V = 1$ liter. (The cavity's and reactant's dimensions are controlled by their diameters (D and d respectively), and their heights (H and h) are adjusted accordingly to maintain the volume.) We consider three reactants specified in Table 3. The seven design variables are allowed to be in the intervals:

$$-35 \le f_x, f_y \le 35 \text{ mm}, -24 \le v_x, v_y \le 24 \text{ mm}, 80 \le d \le 110 \text{ mm}, 75 \le s \le 110 \text{ mm}, 200 \le D \le 300 \text{ mm} \quad (4)$$

The procedure starts with an initial DB of 100 random points in the specified domain. The underlying FDTD model consists of 255,000 to 469,000 cells of 7 mm in air and 2.7 mm in the reactant, and the analysis of the system involves 9,000 time-steps (1.6 to 2.5 min of CPU time).

Here, our optimization algorithm also achieves the objective with different number of FDTD analyses; the optimized design variables are collected in the first lines of Table 4, and corresponding $|S_{11}|$ curves are shown in Fig. 6 – all of them provide at least 99% energy efficiency. One of the main

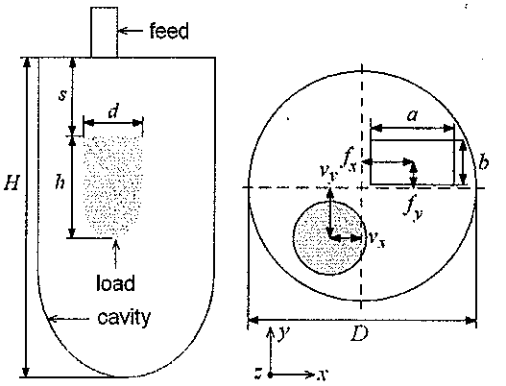

Fig. 5. Schematic view and geometrical parameters of the reactor for microwave-assist organic synthesis.

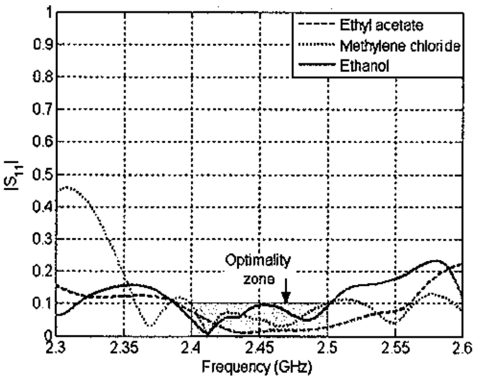

Fig. 6. Reflection coefficient $|S_{11}|$ in the microwave reactors optimized for three different reactants.

Table 3. Material Parameters of the Reactants [8]

Reactant	Dielectric constant, ε'	Electric conductivity, σ (S/m)
Ethyl acetate	6.2	1.181
Methylene chloride	9.1	0.058
Ethanol	24.6	0.147

Table 4. Microwave Chemistry Reactor: Optimized Configurations for Different Reactants

Size of reactor / Reactant	f_x	f_y	v_x	v_y	d	s	D	No of FDTD analyses
1 liter load; Ethanol	27.4	-26.5	-13.8	-6.4	97.2	98.2	236.6	135
1 liter load; Methylene chloride	35.0	-21.1	-2.2	-11.5	92.3	98.6	216.1	339
1 liter load; Ethyl acetate	4.7	-29.3	3.7	-18.8	93.5	94.1	239.9	101
5 liter load; Ethanol	0.5	27.4	-29.3	-30.9	165.5	261.1	350.1	51

challenges of microwave organic chemistry is how to scale up an efficient reaction in a small reactor and synthesize a new substance of a substantially larger volume. Responding to this issue, here we present the solution of the optimization problem for the reactor of the same design, but constructed for $V = 5$ liters. With $H = 513$ mm, the seven design variables are allowed to be in the intervals:

$$-85 \le f_x, f_y \le 85 \text{ mm}, -50 \le v_x, v_y \le 50 \text{ mm}, 159 \le d \le 172 \text{ mm}, 80 \le s \le 300 \text{ mm}, 340 \le D \le 510\text{mm} \quad (5)$$

The procedure starts with an initial DB of 50 random points in the domain (5). The model consisting of 1,157,000 to 2,050,000 cells of 7 mm in air and 3 mm in the reactant require 9,000 time-steps (7.2 to 12.4 min of CPU time) for one FDTD analysis. As the last line of Table 4 shows, the optimal design of the 5-liter reactor is promptly found from only 51 simulations (less than 9 h of CPU time).

Conclusion

The technique of ANN optimization requiring a dramatically reduced number of full-wave simulations has been applied to two complex microwave applicators. 5- to 7-parameter optimization of a loaded microwave oven and a reactor for microwave-assist organic synthesis could take only a few dozen/hundred of FDTD analyses and thus be viable in practical CAD projects.

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