Determination of Optimal Pairs of Radii of Dielectric Samples for Complex Permittivity Measurement of Dispersive Materials

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Abstract— The goal of this work is to find the optimum pair of values of radii of two full height cylindrical samples with the same constitutive properties centrally located in a rectangular waveguide for measurements of the complex dielectric constant. We refer to a pair of values of radii of samples as optimal if the value of measurement uncertainty for the pair is smaller than for other pairs of values. To determine the measurement uncertainty the well known and very powerful Monte Carlo method is employed. Since this method requires a large number of iterations to obtain reliable estimations, the computation of the reflection and transmission coefficients is accelerated by employing an accurate approximation based on a mixed polynomial-rational model.

1. INTRODUCTION

The accurate measurement of the complex dielectric constant is of great importance in electromagnetics, but it is of greater importance medicine. While in electromagnetics uncertainty associated with the the measurement of the dielectric constant can be compensated for by adjusting some adjustable device components, in medicine this, however, may result in, for example, incorrectly made diagnosis. There is a lot of different kinds of measurement techniques such as among others, resonant cavity, transmission line and free space methods. Each of this methods has it's drawbacks and advantages. For example, resonant cavity method allows one to measure the dielectric constant and loss tangent of low loss materials with very high accuracy, but when material under consideration has middle losses the resonant peaks become broader that makes determination of resonant frequency and quality factor less accurate that, in turn, yields higher uncertainty in measurements of the complex dielectric constant. The main drawback of the free space method is that for the accurate measurement of the constitutive properties of materials, the size of the sample must be large enough to neglect diffraction on its sides. One of the main drawbacks of the transmission line methods is lower measurement accuracy as compared to the resonant cavity methods, but at the same time these methods do not require lengthy preparation procedure, that is the case for their resonant counterparts and do not suffer from diffraction on sample sides as free space methods do. For this reason, in the present study we make an attempt to quantify uncertainty measurements of the complex dielectric constant for one of the transmission line methods. The method considered consists in successively placing and making measurements for two dielectric cylindrical samples with different radii. There are two most commonly used methods for quantification of the measurement uncertainty and both are covered in GUM (Guide to Expression of uncertainty in measurements) [2]. The simpler one is the so-called uncertainty propagation method. Unfortunately, validity of this method is restricted only to models that lend themselves to a adequate linear approximation, that makes this method inapplicable to nonlinear models. Another method is the Monte Carlo method that is more powerful, but the main drawback of it, is that it requires powerful computers. For this reason, the uncertainty analysis for measurements of constitutive properties of materials still remains a very time consuming task, because the Monte Carlo method requires a very large number of iterations in order for estimation of the measurement uncertainty to be reliable and because in each of these iterations the inverse scattering problem needs to be solved that, in turn, is a very time consuming task. Since the computational effort required to solve the inverse scattering problem depends directly on the computational time required by the method for the direct scattering problem one needs to find the fastest approach for solving the direct scattering problem. In [3] the reduction in the computation time have been achieved by using piecewise linear interpolation for dependence of the phase and absolute values of the reflection and transmission coefficients on system parameters, separately. Unfortunately, this kind of interpolation proves to be quite inaccurate in vicinity of resonances, that may lead to considerable discrepancy between prediction and actual values of uncertainties. We found that it is more efficient to interpolate the sum and difference of the reflection and transmission coefficients, since for a symmetric obstacle both these quantities have absolute value equal to unity for all real values of the relative dielectric constant that, in turn, means that each pole of this function have the corresponding root such that they are mutually complex conjugate values. Also, these two functions are analytic with respect to the relative complex dielectric constant. Both these properties enable us to use mixed rational-polynomial approximation involving roots and poles of these functions and a polynomial approximating the remaining parts of the functions. The coefficients of these polynomials are found by using least-squares method. In general case, these pairs can be found successively from the derivative of the phase of the functions, but in our case it is simpler and more convenient to determine poles by finding roots of the determinant of a system matrix, since it may be easily proved that the roots of the determinant are the roots of the aforementioned functions as well. Also, in this study we use three normalized quantities, namely, the relative wavelength $\tilde{\lambda}$, relative radius $\tilde{r}$ and relative dielectric constant $\tilde{\varepsilon}$. The main advantage of using normalized quantities is that it leads to reduction in the number of system parameters from four to three and from five to four for dielectric and magnetodielectric materials, respectively. Since in the present study we restrict ourselves to consideration of only dielectric materials we will use only three quantities. Moreover, in case of dielectric samples two of three system parameters have limited range of values, provided the waveguide operates in a single mode regime. Since the functions are analytic they can be completely represented in terms of their poles and roots. As mentioned above, in our case functions have a special structure, that is, its poles and zeros are symmetrically located with respect to the real axis on the complex plane, that simplifies the approximation procedure. Numerical experiments show that, it is sufficient to take only several poles and roots that lie closer on the complex plane to range of interest. This trick allows us to remove rapid changes of function values in the range of interest. The remaining part of the function can be approximated well by a low degree polynomial. The number of poles to be extracted is dependent upon values of other two parameters and length of the interval over which the function is approximated. Both the sum and difference of the reflection and transmission coefficients can be approximated as follows

$$f(\varepsilon) = p(\varepsilon)_{\tilde{\lambda},\tilde{r}} \cdot \prod_{n=1}^{N} \frac{\varepsilon - \tilde{\varepsilon}_n(\tilde{\lambda},\tilde{r})}{\varepsilon - \varepsilon_n(\tilde{\lambda},\tilde{r})} \tag{1}$$

It is obvious that coefficients of the approximating polynomial as well as poles and roots are functions of $\tilde{\lambda}$ and $\tilde{r}$. Fortunately, this functions are monotonous and do not exhibit any rapid changes, that is, they can be accurately approximated using piecewise linear approximations.

2. SOLUTION OF THE DIRECT SCATTERING PROBLEM

Despite the fact, that many approaches for determination of the reflection and transmission coefficients over the last several decades, not all of them provide results with reasonable accuracy and the same time show rapid convergence. From many approaches that have been proposed over the last several decades [4–13], we have chosen that proposed by Sahalos et al. [11] as it provides reasonably accurate results and at the same time shows very rapid convergence. This approach is based upon expressing the fields in the homogenose regions in terms of series of solutions of the homogenous Helmholtz equation. Such kind of representation allows one to solve boundary problem on the surface of the post analytically that, in turn, considerably reduce overall computational effort. The first approach of this kind have proposed by Nielsen [12], but it converged only for cylindrical samples with quite small electrical radius. Sahalos et al. have overcome this limitation by replacing the rectangular interaction region with the circular one, where the center of the circular interaction region coincides with the axis of the post and its radius is equal to half the width of the broader wall of the waveguide. Later it was found that applying numerical integration on the surface of the interaction region instead of point matching procedure yields faster convergence [13].

In order to simplify solution problem under consideration, we need to make several assumptions. The first one is that the walls of the rectangular waveguide are treated as perfectly conducting, which is the case since walls of waveguides are typically covered by highly conductive material. Also we assume that only dominant mode may propagate in the waveguide and all other modes don't take part in power transfer and decay very rapidly with distance from the sample. In order to solve the problem we divide the waveguide into three separate regions as depicted in Figure 1.

In region I and III scattered fields are represented in terms of waveguide modes.

$$E_y^I = \sum_{m=1}^{\infty} A_m \cos\frac{m\pi x}{a} e^{-jk_m z} \tag{2}$$

$$E_y^{III} = \sum_{m=1}^{\infty} B_m \cos\frac{m\pi x}{a} e^{jk_m z} \tag{3}$$

In region II fields and inside the cylindrical sample fields are represented in terms of cylindrical waves.

$$E_y^{II} = \sum_{n=0}^{\infty} \left(C_n J_n\left(2\pi\tilde{\lambda}\tilde{r}\right) + D_n Y_n\left(2\pi\tilde{\lambda}\tilde{r}\right)\right)\cos(n\cdot\varphi) \tag{4}$$

$$E_y^{p} = \sum_{n=0}^{\infty} E_n J_n\left(2\pi\tilde{\lambda}\tilde{r}\tilde{\varepsilon}\right)\cos(n\cdot\varphi) \tag{5}$$

where $k_m = k_o\sqrt{1-\frac{4}{\tilde{\lambda}^2}}$ — is the waveguide wavenumber, k_o — wavenumber in free space. Expressions for corresponding magnetic fields in these regions may be obtained by using the second Maxwell's equation.

Enforcing boundary conditions on the surface of the post as well as taking the advantage of the mutual orthogonality of cylindrical waves with respect to azymuthal coordinate and eliminating the unknown constants, the expression for the electric field in region II may be written as follows

$$E_y^{II} = \sum_{n=0}^{\infty} \left(C_n J_n\left(2\pi\tilde{\lambda}\tilde{r}\right) + \frac{\alpha_n}{\beta_n} Y_n\left(2\pi\tilde{\lambda}\tilde{r}\right)\right)\cos(n\cdot\varphi) \tag{6}$$

where

$$\alpha_n = J_n(2\pi\tilde{\lambda}\tilde{r}\tilde{\varepsilon})J_n'(2\pi\tilde{\lambda}\tilde{r}) - \tilde{\varepsilon}J_n'(2\pi\tilde{\lambda}\tilde{r}\tilde{\varepsilon})J_n(2\pi\tilde{\lambda}\tilde{r}) \tag{7}$$

$$\beta_n = \tilde{\varepsilon}Y_n(2\pi\tilde{\lambda}\tilde{r})J_n'(2\pi\tilde{\lambda}\tilde{r}\tilde{\varepsilon}) - Y_n'(2\pi\tilde{\lambda}\tilde{r})J_n(2\pi\tilde{\lambda}\tilde{r}\tilde{\varepsilon}) \tag{8}$$

In order to obtain a system of linear equations for unknown expansion coefficients, one has to enforce the boundary conditions on the surface of the interaction region S. Since in this case the boundary value problem cannot be solved analytically we employ the variational approach, that is, we formulate boundary conditions for the tangential components of the electric and magnetic fields on the imaginary surface (interaction region) in the weak form. In other words, we require that the projection of the difference between field representations on both sides of the interaction region S upon a properly chosen set of test functions equal to zero almost everywhere. There are many different sets of testing functions, but in the present case the most suitable choice is the following set of trigonometric functions satisfying periodic boundary conditions $\cos p\varphi$ (where $p = 1, 2, ..., M$).

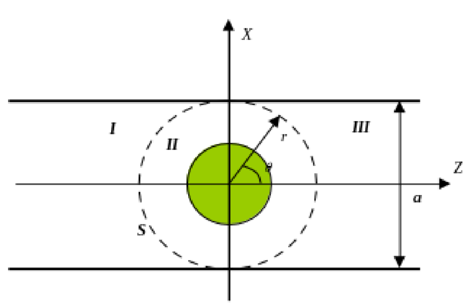

Figure 1: The rectangular waveguide containing the cylindrical dielectric sample.

3. DISCUSSION

It is well known that the analytical solution of the inverse scattering problems is possible only for structures under consideration, having very simple problem geometries. Even when the direct scattering problem may be solved analytically it not always possible to solve the corresponding inverse problem analytically without any approximations. Due to this fact, we will use one of the most common numerical procedures that consist in converting an inverse problem to an equivalent numerical minimum finding problem, i.e., optimization problem. An objective function is chosen as the distance between calculated and measured values of S parameters.

$$Q(f) = \sqrt{\sum_{m=1}^{2}\sum_{n=1}^{2}\left(S^{s}_{mn} - S^{m}_{mn}\right)} \tag{9}$$

where — is $Q(f)$ the objective function; S^{m}_{mn} — measured values of scattering matrix entries; S^{s}_{mn} — values of the scattering parameters obtained by solving the corresponding direct scattering problem. Since the objective function consists of a sum of the squares, it takes minimum value when values of the coordinates correspond to the solution of the inverse scattering problem. There are many algorithms that may be employed for finding the global minimum of objective functions, but after a number of numerical investigations we found that for solving the problem under consideration a simple pattern search method [14], the Nelder-Mead simplex method [15], as well as its improved versions are the best candidates. One of the most widely used approaches for measurements of the dielectric constant is the so-called multi-frequency approach. It consists in making measurements of scattering data at, at least, two different frequencies in order for a solution to be unique as it is obvious that when measurements are made only at one particular frequency the scattering coefficients may take the same value at different values of the complex permittivity. Nevertheless, this multi-frequency method cannot be applied in a case of highly dispersive materials, where constitutive parameters vary very rapidly with frequency. In this case we need to employ another measurement method, which not only ensures uniqueness of the solution, but also allows one to make all measurement at some fixed frequency. One such method is to make measurements of two samples with different values of some geometric parameters at a fixed frequency value. Another, also, widely used in practice measurement method is to make measurements at fixed frequency, but for different positions of a movable short circuit, terminating one of the ends of the waveguide or transmission line section. The latter approach, however, has a limitation, namely, the absolute value of the reflection coefficient is always equal to unity for samples made from lossless materials. In other words, the only quantity we can measure is the phase of the reflection coefficient. In the present study we employ the former one while the latter one will be the subject of the forthcoming studies.

4. NUMERICAL RESULTS

It is convenient to represent measurement process in terms of model with its input and output quantities. There are uncountably many factors that affect the accuracy of measurements, but in practice it suffice to take into consideration only those that make the most significant contribution to the overall accuracy. Among the factors belonging to these category are the limited resolution, residual systematic error, connection mismatch, and geometrical imperfections of the sample, such as a small shift in the position of the sample and the accuracy of the measurement of the radius of the cylindrical sample. Typically, the uncertainty of the measurable quantity is dependent upon value of model parameters. In other words it may be possible that for some optimal combinations of values of these parameters the standard uncertainty $u(\varepsilon)$ of the output quantity will be smaller than for all other combinations.

In this paper we consider the dependence of the standard uncertainty $u(\varepsilon)$ of the output quantity upon two system parameters, namely, the radii of the cylindrical samples. In order to find optimal values of the radius of the sample we estimate the standard uncertainty in measurement of the dielectric permittivity by using the Monte Carlo method. According to standards, probability distributions for input quantities of the model are assigned according to the maximum entropy principle. In our case we take into account uncertainties due to the frequency accuracy, imperfect measurement of the radii of the samples and scattering data. Also, we assume that errors associated with measurements of scattering data are distributed according to the normal distribution, while those associated with frequency and dimensional parameter measurements are distributed according

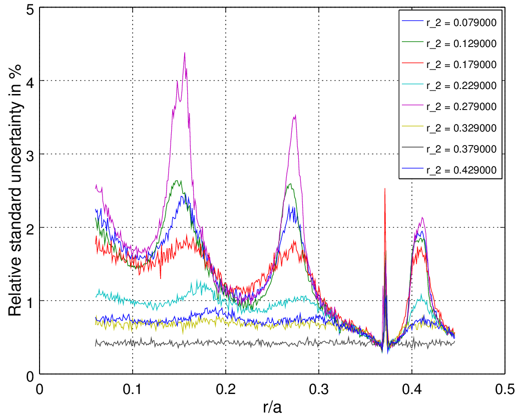

Figure 2: The standard uncertainty $u(\varepsilon)$ of the dielectric constant versus the relative radius of the post $\tilde{r} = r/a$, measuring absolute values the reflection and transmission coefficients with the following values of standard uncertainties of input quantities: $u(|R|) = 0.02\%$, $u(\arg(R)) = 3\,\text{degrees}$, $u(r) = 0.01\,\text{mm}$, $u(f) = 1.0\,\text{MHz}$.

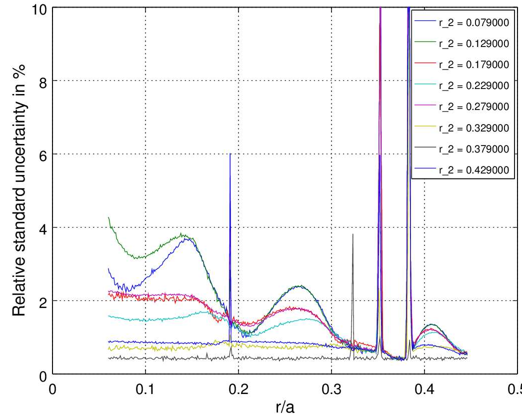

Figure 3: The standard uncertainty $u(\varepsilon)$ of the dielectric constant versus the relative radius of the post $\tilde{r} = r/a$, measuring absolute value and phase of the reflection coefficient with the following values of standard uncertainties of input quantities: $u(|R|) = 0.02\%$, $u(\arg(R)) = 3\,\text{degrees}$, $u(r) = 0.01\,\text{mm}$, $u(f) = 1.0\,\text{MHz}$.

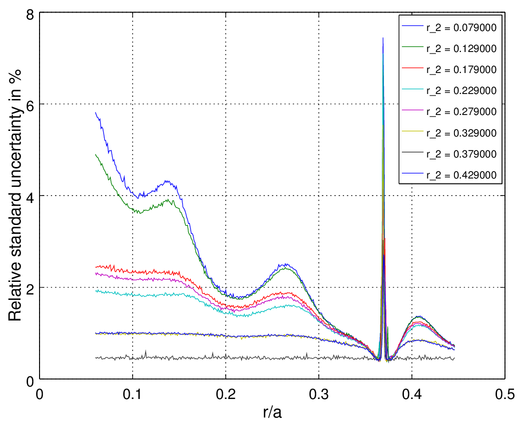

Figure 4: The standard uncertainty $u(\varepsilon)$ of the dielectric constant versus the relative radius of the post $\tilde{r} = r/a$, measuring both the absolute value and phase of the transmission coefficient with the following values of standard uncertainties of input quantities: $u(|R|) = 0.02\%$, $u(\arg(R)) = 3\,\text{degrees}$, $u(r) = 0.01\,\text{mm}$, $u(f) = 1.0\,\text{MHz}$.

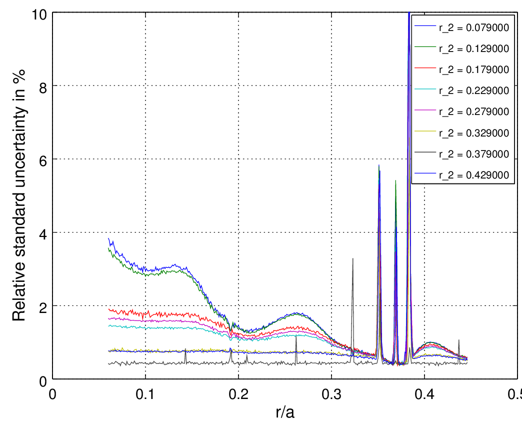

Figure 5: The standard uncertainty $u(\varepsilon)$ of the dielectric constant versus the relative radius of the post $\tilde{r} = r/a$, measuring both the absolute value and phase of the reflection and transmission coefficients with the following values of standard uncertainties of input quantities: $u(|R|) = 0.02\%$, $u(\arg(R)) = 3\,\text{degrees}$, $u(r) = 0.01\,\text{mm}$, $u(f) = 1.0\,\text{MHz}$.

to uniform distribution. Normally distributed random numbers are generated by using uniformly distributed random numbers that are, in turn,generated by the pseudo-random number generator and by applying Box-Muller transform. In this study we assume that the systematic part of measurement uncertainty is very small, which is the case, provided proper calibration procedures have been performed before measurements.

5. CONCLUSION

To find values of the radius of the cylindrical sample at which the value of measurement error has the smallest influence on the accuracy of determination of the dielectric permittivity, we have applied the Monte Carlo method with a total of 10000 iterations. All graphs are obtained for system with following parameter values $\tilde{\lambda} = 0.8$ and $\tilde{\varepsilon} = 5.0$. As have been expected, the numerical results show that the uncertainty of measurement of the dielectric permittivity varies with the value of the relative radius of the sample r/a. It is seen in Figures 2–5 that there are many optimal pairs of values of radii of samples under investigation, provided at least one of these values belongs to the range of $\tilde{r}$ where the reflection and transmission coefficients as functions of $\tilde{r}$ have very high steepness. Unfortunately, the greater is the steepness, the shorter is the optimal range of $\tilde{r}$ which makes it very difficult if not impossible to produce sample such that its radius is in the desired range of values.

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