Reconstruction of Complex Permittivity of Dispersive Materials with FDTD Modeling Controlled by Neural Networks

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ABSTRACT

The paper is focused on some practical aspects of a new efficient technique for determining the dielectric properties of materials. Complex permittivity is found by an artificial neural network designed to control 3D FDTD computation of *S*-parameters and to process their measurements. The method is cavity-independent and applicable to samples of arbitrary configurations (as long as the geometry is adequately represented in the FDTD model). We consider a two-port approach which exploits the real and imaginary parts of the reflection and transmission coefficients at the frequency of interest and is capable of handling frequency-dependent media parameters. Numerical testing demonstrates a high accuracy of the computational part of the method (less than 2% for dielectric constant and the loss factor varying in very wide ranges). It is shown that when processing the measured *S*-parameters, the developed network is capable of efficiently generalizing and reconstructing complex permittivity even from experimental data which are numerically inconsistent with the modeling data used for network training. Special modeling tests validate a satisfactory level of accuracy in permittivity reconstruction for salt water, ethylene glycol-water mixture, denatured alcohol and acetone at 915 MHz.

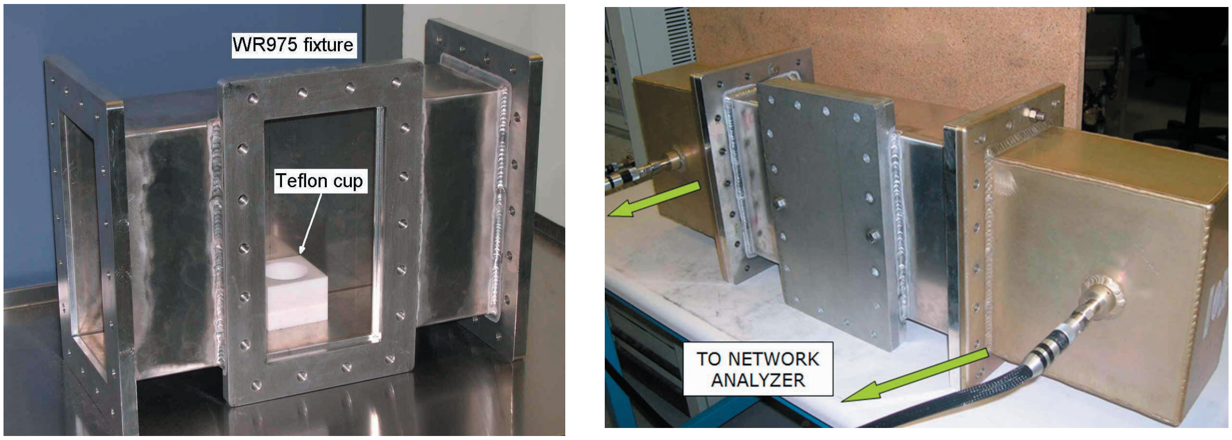
INTRODUCTION

Recently, with the remarkable progress of computational resources, computer-aided design has become a valuable component in developing systems of microwave power engineering. Knowledge of complex permittivity ($\varepsilon = \varepsilon' - i\varepsilon''$) of dielectric materials involved in an application is critical for creating an adequate model and thus for successful system design. However, the dielectric constant ε' and the loss factor ε'' are not always available. The lack of data regarding realistic materials to be processed in microwave applicators motivates the development of efficient and practical techniques for determining complex permittivity.

Since the design of a microwave system is supposed to be motivated by modeling, it is logical to make a related numerical simulator involved in determination of material parameters – anyway, ε' and ε'' cannot be measured, but can be calculated given the data on some measurable characteristics. In our previous papers [1, 2], we have reported the development of an innovative method of permittivity reconstruction. This method deals with an arbitrary cavity containing an arbitrarily shaped sample of material in question. Its complex permittivity is found using an artificial neural network procedure designed to control 3D FDTD computation of *S*-parameters of this system and to process the results of their measurements.

METHOD

This paper presents the outcome of further practice-oriented development of this approach. This time, it is implemented with a transmission-line-type fixture (Figs. 1 and 2) and exploits the magnitude and phase of the



(a) **(b)**

Fig. 1. The WR975-based two-port fixture with the Teflon cup (a container accommodating liquids to be tested) (a) and the assembled experimental setup (b)

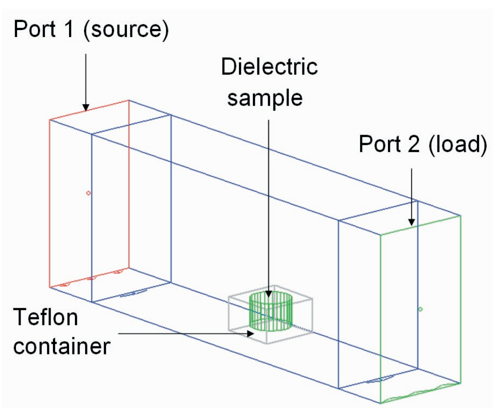


Fig. 2. 3D view of the FDTD model.

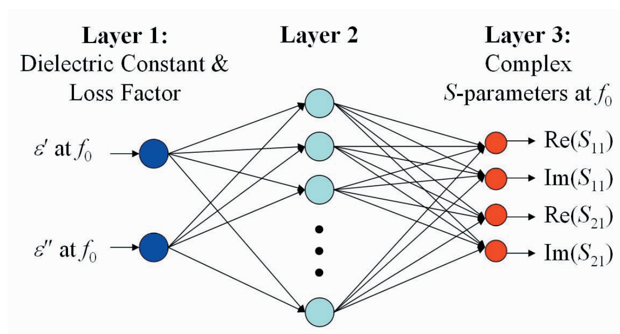
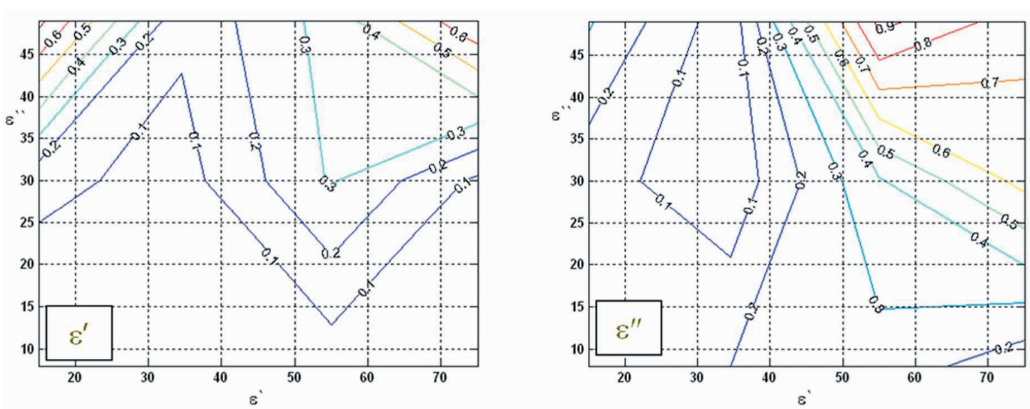
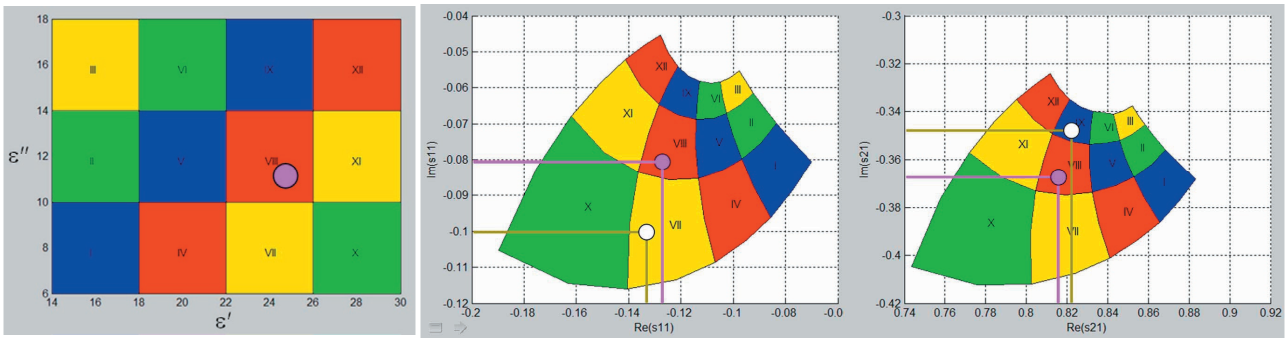


Fig.3. The RBF network employed in the method.



(a) (b)

Fig. 4. Accuracy of reconstruction of dielectric constant (a) and the loss factor (b) – numerical tests with 36 point databases for sub-domains Δε′ = Δε″ = 10 on the ε-plane.



(a) (b) (c)

Fig. 5. A domain near an unknown (ε′, ε″)-point in the ε-plane (a) and this domain's maps in the S_{11}-plane (b) and S_{21}-planes (c); measured (o) and reconstructed points ( ) for Sample DA (see Table 1).

reflection and transmission coefficients (or, in terms of *S*-parameters, $|S_{11}|$, $<S_{11}$, $|S_{21}|$, $<S_{21}$) at the frequency of interest f_0. A rectangular (70×70×50 mm) Teflon block with a cylindrical cutout (radius 25 mm, height 40 mm) suitable for holding liquids is placed on the bottom (i.e., narrow waveguide wall) of the cavity. A two-port approach allows us to work with a set of *S*-parameters at one frequency (instead of several points of a $|S_{mn}|$ frequency response in the one-port scheme [1]) and thus to deal with dispersive materials. The "vertical" orientation of the waveguide fixture is introduced in order to arrange for the air-sample media interface parallel to the direction of the electric field and thus to make the fixture's parameters not sensitive to a possible uncertainty in the interface's location.

The radial basis function (RBF) network used in this work is shown in Fig. 3. Data for training is generated by an FDTD model (built with the use of *QuickWave-3D*) which precisely reproduces the fixture and contains, depending on the dielectric constant of the sample, from ~60 to 265 thousand rectangular cells using ~6 and 25 MB of RAM respectively. Detailed characterization of this network is given in [2].

RESULTS & DISCUSSION

Systematic numerical testing of the network performance has shown that the computational part of the method is highly accurate. For example, using the databases of 25 to 64 points in the sub-domains $\Delta\varepsilon' = \Delta\ \varepsilon'' = 10$ on the complex permittivity plane, dielectric constant and the loss factor are reconstructed with errors less than 1-2% along most of the ε-plane. Typical graphs illustrating the results of these tests are shown in Fig 4.

On the other hand, when *S*-parameters supplied to the network are taken not from the model but from the related measurements, a numerical dispersion may occur making the network "feel" that the experimental data are inconsistent with the training ones. This effect is purely numerical in nature rather than resulting from the "quality" of the model and has received special treatment. The measures taken to enhance the generalization of the network and make it capable of handling data of this sort include an adjustment of the model in accordance with calibration of the experimental setup (with subsequent generation of the database), optimization of the RBF radius, and improvement of smoothness of data with the use of ridge regression [3].

Electromagnetic characteristics of the fixture strongly depend on complex permittivity of the tested material, so the related FDTD models should be appropriately "tuned" for different values of ε′ and ε″. This means that it is not possible to operate the method using the same model and a single (sufficiently large) database for the entire ε-plane. Therefore, we have developed a special two-step procedure allowing the user to roughly locate the position of the unknown (ε′, ε″)-point and then to build a relatively small database in its neighborhood. This procedure also helps keep the numerical dispersion under control.

Fig. 5 illustrates the network generalization achieved upon implementation of all these steps. The set of experimental data Re(S_{11}), Im(S_{11}), Re(S_{21}), and Im(S_{21}) defines the points representing the (ε′, ε″)-pair in the S_{11}- and S_{21}-planes, and these points appear to be inconsistent with the maps generated on these planes with the use of modeling data – indeed, the points are located in different sub-domains (S_{11} in VII and S_{21} in IX). However, the neural network successfully processes the measured data and reconstructs the (ε′, ε″)-point which, being plotted back on the S_{11}- and S_{21}-planes, is represented by the points in sub-domain VIII.

Table 1. Reconstructed Complex Permittivity of Tested Liquids at 915 MHz

Sample	Material	Temp., C	ε′	ε″
SW	Salt water (3.88% NaCl by weight)	22.5	66.0	139.0
EGW	Ethylene glycol (68%) + water (32%)	22.7	60.8	13.1
DA	Denatured alcohol	21.0	24.7	10.3
AC	Acetone	22.5	20.1	0.44

Table 2. Validation of the Results in Table 1 – Scenario with Half a Sample

Sample	*S*-Parameter	Re(S_{11})	Im(S_{21})	Re(S_{21})	Im(S_{21})
SW	Measured	-0.036	-0.030	0.923	-0.306
	Modeled (with reconstructed ε)	-0.033	-0.028	0.924	-0.306
EGW	Measured	-0.040	-0.069	0.905	-0.340
	Modeled (with reconstructed ε)	-0.041	-0.073	0.903	-0.345
DA	Measured	-0.023	-0.038	0.935	-0.323
	Modeled (with reconstructed ε)	-0.023	-0.039	0.934	-0.323
AC	Measured	-0.015	-0.035	0.946	-0.321
	Modeled (with reconstructed ε)	-0.013	-0.038	0.945	-0.322

Table 1 contains the values of reconstructed complex permittivity obtained with the use of our method for four sample liquids – two artificially made and two readily available. To validate these results, an FDTD model has been run with the determined ε′ and ε″, but for an alternative geometry – the Teflon cup is half-full with the liquid. The real and imaginary parts of *S*-parameters were measured and compared with the modeled results (see Table 2). The fact that they differ by no more than 0.005, suggests that our method reconstructs complex permittivity with an accuracy absolutely sufficient for modeling purposes.

CONCLUSIONS

It has been demonstrated that the novel neural-network-based technique of permittivity reconstruction is viable and efficient – the method successfully determines complex permittivity of series of diverse liquids at 915 MHz. In general, the technique is frequency- and cavity-independent, applicable to the sample/fixture of arbitrary configuration, and capable of handling highly frequency-dependent media parameters. For materials which can take some predefined form, computational cost of the method is very insignificant. A full-wave modeling tool and the controlling neural network procedure involved allow for much flexibility in the practical implementation of the method.

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