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Optimal parameters of experiment for determining dielectric constant of a layer in a rectangular waveguide

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Abstract

The inverse problem is considered of reconstructing real permittivity of a plane-parallel layer in a perfectly conducting rectangular waveguide from experimental data using explicit expression for the scattering matrix. This problem is incorrect because of the presence of self-intersection points on the scattering coefficients curves on the complex plane. It is shown that the traditional multi-frequency method of measurements applied in vector network analyzers can be justified using the fact that the algorithm for processing the measurement results that employs least squares becomes stable if the number of frequencies is large enough.

1 Problem settings

We study the problem of determining permittivity of a dielectric inclusion (a layer) in a standard rectangular waveguide (Fig. 1) from the elements of the scattering matrix or the transmission coefficient of the principal waveguide mode.

Figure 1. Rectangular waveguide with a layer [1].

The measurement data registered at the layer boundaries have the form [2]

$$S_{11}^{(layer)} = \frac{(1 - Z^2)\Gamma}{1 - \Gamma^2 Z^2}, \quad (1)$$

$$S_{12}^{(layer)} = \frac{(1 - \Gamma^2)Z}{1 - \Gamma^2 Z^2}, \quad (2)$$

while the values of the scattering matrix elements measured at the waveguide flanges are

$$S_{12}^{(wg, layer)} = S_{12}^{(layer)} Z_1 Z_2, \quad S_{11}^{(wg, layer)} = S_{11}^{(layer)} / (Z_1)^2,$$

which are calculated by the complex amplitude of the harmonic Maxwell's equations solution

$\mathbf{E}(\mathbf{r}, t) = \hat{\mathbf{E}}(\mathbf{r})e^{-i\omega t}$, $\omega = 2\pi f$, f is the source frequency, satisfying the condition of single-mode waveguide. Here

$$\Gamma = (t_\varepsilon(f) - 1)/(t_\varepsilon(f) + 1), \quad t_\varepsilon(f) = k_\varepsilon^{(z)}(f)/k_1^{(z)}(f),$$

$$k_\varepsilon^{(z)}(f) = (k_\varepsilon^2(f) - (k^{(x)})^2)^{1/2},$$

$$k_1^{(z)}(f) = (k_1^2(f) - (k^{(x)})^2)^{1/2},$$

$$k_\varepsilon^2(f) = \varepsilon k_1^2(f), \quad k_1^2(f) = \omega^2 \varepsilon_0 \mu_0, \quad k^{(x)} = \pi/a,$$

a is the waveguide width, $d^{(wg)}$, $d^{(layer)}$ are the waveguide and layer lengths, d_1 , d_2 are the distances between the ports (points of source and field measurements) and the layer, $d^{(wg)} = d^{(layer)} + d_1 + d_2$, $\varepsilon = \varepsilon^{(layer)}$ is the layer relative dielectric constant, and ε_0 is the dielectric constant of vacuum;

$$Z_1(f) = e^{ik_1^{(z)}(f)d_1}, \quad Z_2(f) = e^{ik_1^{(z)}(f)d_2},$$

$$Z_0^{(wg)}(f) = e^{ik_1^{(z)}(f)d^{(wg)}}, \quad Z_0^{(layer)}(f) = e^{ik_1^{(z)}(f)d^{(layer)}},$$

$$Z = Z^{(layer)}(f) = e^{ik_\varepsilon^{(z)}(f)d^{(layer)}}$$

are the phase shift values inside the waveguide.

Introduce the transmission coefficient of the principal mode in a single-mode perfectly conducting rectangular waveguide scattered by the dielectric layer

$$F(\varepsilon, f) = S_{12}^{(wg, layer)}(\varepsilon, f) / S_{12}^{(wg)}(f). \quad (3)$$

Here $S_{12}^{(wg, layer)}$ is the element of the scattering matrix corresponding to the transmission of the wave through the waveguide containing the dielectric layer and $S_{12}^{(wg)} = Z_0^{(wg)}$ is the corresponding element of the scattering matrix for an empty waveguide.

In the presence of a dielectric insert of arbitrary shape the measurement results change due to the occurrence, in

addition to the harmonic waves in the principal mode, a countable number of evanescent waves (standing waves that exponentially decay along the axis of the waveguide). The transmission coefficient of the principal mode through a dielectric layer can be found as

$$F(\varepsilon, f) = Z_0^{(layer)}(f) / g(\varepsilon, f), \quad (4)$$

where

$$g(\varepsilon, f) = c_\varepsilon(f) + iH(t_\varepsilon(f))s_\varepsilon(f), \quad (5)$$

$$s_\varepsilon(f) = \sin(k_\varepsilon^{(z)}(f)d^{(layer)}), \quad (6)$$

$$c_\varepsilon(f) = \cos(k_\varepsilon^{(z)}(f)d^{(layer)}),$$

and $H(x) = 0.5(x + 1/x)$, $x > 0$.

Formulas (4)–(6) constitute the exact solution of Maxwell's equations for the transmission coefficient of the principal mode; a recurrent formula generalizing (4) to the case of a multilayer inclusion is given in [4]. They are equivalent to expressions (2), (3) known since 1970 [2]. Representations (1), (2) were used in the NRW method [2, 3] according to which complex parameters of a slab in free space and in a waveguide are determined explicitly from the scattering matrix elements $S_{11}^{(layer)}$, $S_{12}^{(layer)}$ using the expressions

$$\varepsilon_1 = (c_2 / c_1)^{1/2}, \quad \mu_1 = (c_1 c_2)^{1/2},$$

$$c_1 = (1 + \Gamma)^2 / (1 - \Gamma)^2, \quad c_2 = -\left(c \ln Z / \omega d^{(layer)}\right)^2,$$

$$V_1 = S_{12}^{(layer)} - S_{11}^{(layer)}, \quad V_2 = S_{12}^{(layer)} + S_{11}^{(layer)},$$

$$X = (1 - V_1 V_2) / (V_1 - V_2),$$

$$\Gamma = X \pm (X^2 - 1)^{1/2}, \quad Z = (V_1 - \Gamma) / (1 - V_1 \Gamma).$$

Due to the properties of function $\ln z$ of a complex variable this algorithm has ambiguity. The ambiguity was removed in [3] using multi-frequency measurements and finite-difference approximation of the derivative of the phase Z with respect to f which is monotonic with respect to variable ε on certain intervals of its variation. Another remaining difficulty of this algorithm, however, is that it is not stable due to instability of approximate differentiation employing inaccurate data.

In the next sections we discuss an alternative to the NRW method for determining the value of the dielectric constant of an inclusion solely from the transmission coefficient (3), (4). An advantage of the developed approach is caused by the convenience of measurements when the phase shifts and exact values of the distances between the ports and the layer are not used.

2 Algorithms of Experimental Data Processing

Introduce the vectors

$$\mathbf{f} = \{f_i\}_{i=1, \dots, N_{\text{exp}}} \in \mathbb{R}^{N_{\text{exp}}}, \quad \mathbf{F}^{\text{exp}} = \{F_i^{\text{exp}}\}_{i=1, \dots, N_{\text{exp}}} \in \mathbb{C}^{N_{\text{exp}}}$$

of the frequency and complex-valued measurement data of N_{exp} experiments. Consider the equation

$$\mathbf{g}(\varepsilon^{(layer)}, \mathbf{f}) = \mathbf{g}^{\text{exp}} \quad (7)$$

for the (unknown) dielectric constant of the layer $\varepsilon^{(layer)} \geq 1$, where

$$\mathbf{g}(\varepsilon, \mathbf{f}) = (g(\varepsilon, f_1), \dots, g(\varepsilon, f_{N_{\text{exp}}}))$$

with g defined in (5), (6),

$$\mathbf{g}^{\text{exp}} = (g_1^{\text{exp}}, \dots, g_{N_{\text{exp}}}^{\text{exp}}),$$

$$g_i^{\text{exp}} = Z_0^{(layer)}(f_i) / F_i^{\text{exp}}, \quad i = 1, \dots, N_{\text{exp}}.$$

We formulate inverse problems that constitute different permittivity reconstruction scenarios. To this end, let

$$\Omega^{(\varepsilon)} = \{\varepsilon : \varepsilon \geq 1\}, \quad \Omega_E^{(\varepsilon)} = \{\varepsilon : 1 \leq \varepsilon \leq E\},$$

and by

$$G(\mathbf{f}, \Omega^{(\varepsilon)}) = \{\mathbf{g}(\varepsilon, \mathbf{f}) \in \mathbb{C}^{N_{\text{exp}}}, \varepsilon \in \Omega^{(\varepsilon)}\}$$

denote the set of values of function $\mathbf{g}(\varepsilon, \mathbf{f})$ for the selected frequency vector $\mathbf{f}$ (a curve on the complex plane).

Problem 1. Find a real $\varepsilon^{(layer)} \in \Omega^{(\varepsilon)}$ satisfying the relation (7) for a given complex vector $\mathbf{g}^{\text{exp}} \in G(\mathbf{f}, \Omega^{(\varepsilon)})$ with the selected frequency vector $\mathbf{f}$.

Problem 2. Find a real $\varepsilon^{(layer)} \in \Omega^{(\varepsilon)}$ satisfying the relation (7) for a given complex vector $\mathbf{g}^{\text{exp}} \in \mathbb{C}^{N_{\text{exp}}}$ with the selected frequency vector $\mathbf{f}$.

Check the fulfillment of the correctness condition for these problems; namely, the existence and uniqueness of solution and its continuous dependence on the input data. Problem 1 describes a perfect experiment exactly corresponding to the mathematical model, it is solvable by the definition of the set $G(\mathbf{f}, \Omega^{(\varepsilon)})$. However, its uniqueness may be violated. In fact, if $N_{\text{exp}} = 1$ for any chosen frequency the solution is not unique due to the existence of a countable set $\{\varepsilon_m, m = 1, \dots\}$, satisfying the relation $\sin(k_{\varepsilon_m}^{(z)}(f)d^{(layer)}) = 0$ that specifies self-intersections points of curve $G(f, \Omega^{(\varepsilon)})$ (see Fig. 2).

Using *a priori* information about $\varepsilon^{(layer)}$ we can achieve the uniqueness of solution by adjusting domain $\Omega^{(\varepsilon)}$ and a frequency range $[f_1, f_2]$. However, the formally correct problem may be ill-conditioned in the vicinity of the points mentioned above where the parameter values are such that the quantity $\sin(k_{\varepsilon}^{(z)}(f)d^{(layer)}) \approx 0$ in the denominator.

When the number of measurements N_{exp} is large enough, the solution to Problem 1 exists and is unique. In fact, the proposition in Section 3 below demonstrates that $\mathbf{g}(\varepsilon, \mathbf{f})$

becomes a one-to-one vector-function of real variable ε for a fixed set of frequency values $\mathbf{f}$.

Problem 2 simulates processing noisy experimental data. This problem is also incorrect; namely, in addition to the presence of self-intersection points noted for Problem 1, it may be unsolvable. Indeed, in actual experiments, it is typical that $\mathbf{g}^{\text{exp}} \notin G(\mathbf{f}, \Omega^{(\varepsilon)})$ because the set (a curve) has the zero measure on the complex plane.

To obtain an approximate solution of incorrectly posed Problem 2, it is necessary to replace it with another one which will be well-posed and such that its solution approximates the sought solution of Problem 1 when the measurement error decreases.

Figure 2. The branches of the curve $G(f, \Omega^{(\varepsilon)})$, $f = 9.25$ GHz, $\Omega^{(\varepsilon)} = \{\varepsilon : 1.0 \leq \varepsilon \leq 9.0\}$, corresponding to $\varepsilon \in \Omega_1^{(\varepsilon)} = (2.05, 2.13)$ (purple), $\varepsilon \in \Omega_2^{(\varepsilon)} = (3.06, 3.12)$ (green), their intersection point $g(\varepsilon_1, f) = g(\varepsilon_2, f)$, $\varepsilon_1 = 2.09 \in \Omega_1^{(\varepsilon)}$, $\varepsilon_2 = 3.12 \in \Omega_2^{(\varepsilon)}$, $\mathbf{g}^{\text{exp}}$.

3 One-to-One Correspondence

One can show that the transition from a single-frequency experiment to a multi-frequency one improves the properties of the inverse problem providing its unique solvability. The following statement is valid:

Proposition

- If $N_{\text{exp}} = 1$ and E is large enough, there is no one-to-one correspondence between $\Omega_E^{(\varepsilon)}$ and $G(f, \Omega_E^{(\varepsilon)})$.
- For any $E > 1$ there is a number N_E such that for $N_{\text{exp}} > N_E$ there is one-to-one correspondence between $\Omega_E^{(\varepsilon)}$ and $G(\mathbf{f}, \Omega_E^{(\varepsilon)})$ (see Fig. 3):

$$\mathbf{g}(\varepsilon_1, \mathbf{f}) = \mathbf{g}(\varepsilon_2, \mathbf{f}) \rightarrow \varepsilon_1 = \varepsilon_2.$$

Proof

- The one-to-one correspondence of the sets specified in part a is violated because of the existence of self-intersection points

$$\varepsilon_m = \frac{1}{\omega^2 \varepsilon_0 \mu_0} \left(\frac{\pi^2 m^2}{(d^{(\text{layer})})^2} + (k^{(x)})^2 \right), \quad m = 1, \dots,$$

of the curve $G(f, \Omega_E^{(\varepsilon)})$ at which

$$s_{\varepsilon_m}(f) = 0, \quad |g_{\varepsilon_m}(f)| = 1.$$

- (reductio ad absurdum). Let $N_{\text{exp}} > 1$, and $\varepsilon_1, \varepsilon_2$ be the values of the dielectric constant of the layer such that $1 \leq \varepsilon_1 < \varepsilon_2 \leq E$,

$$\|\mathbf{g}(\varepsilon_1, \mathbf{f}) - \mathbf{g}(\varepsilon_2, \mathbf{f})\|_{C^{N_{\text{exp}}}} = 0.$$

From the properties of functions $H(x)$ and $t_\varepsilon(f)$ it follows that $s_{\varepsilon_1}(f_i) = 0$ for $i = 1, \dots, N_{\text{exp}}$, that is, $\{f_i\}_{i=1, \dots, N_{\text{exp}}}$ belongs to the set of zero points of function $s_{\varepsilon_1}(f)$, and their number in the frequency range $[f_1, f_2]$ does not exceed

$$N_E = 2 \left(E \varepsilon_0 \mu_0 (f_2^2 - f_1^2) \right)^{1/2} d^{(\text{layer})} + 1,$$

so $\varepsilon_1 = \varepsilon_2$ if $N_{\text{exp}} > N_E$. ■

Figure 3. a. The vectors

$$\begin{aligned} & \left(g(\varepsilon_{1,l}, f_1), \dots, g(\varepsilon_{1,l}, f_{N_{\text{exp}}}) \right), \\ & \left(g(\varepsilon_{2,l}, f_1), \dots, g(\varepsilon_{2,l}, f_{N_{\text{exp}}}) \right), \end{aligned}$$

$$N_{\text{exp}} = 5, \quad f_1 = 9.25 \text{ GHz}, \quad f_{N_{\text{exp}}} = 9.2504 \text{ GHz},$$

$$\varepsilon_{1,l} \in \Omega_1^{(\varepsilon)}, \quad \varepsilon_{2,l} \in \Omega_2^{(\varepsilon)}, \quad l = 1, \dots,$$

$$\varepsilon_{1,3} = \varepsilon_1 = 2.09, \quad \varepsilon_{2,4} = \varepsilon_2 = 3.12 \text{ (Fig. 2)},$$

- $g(\varepsilon_1, f_1) = g(\varepsilon_2, f_1)$, $g_{\varepsilon_1}(f_i) \neq g_{\varepsilon_2}(f_i)$, $i = 2, \dots, N_{\text{exp}} \rightarrow \mathbf{g}(\varepsilon_1, \mathbf{f}) \neq \mathbf{g}(\varepsilon_2, \mathbf{f})$.

Thus, at any frequency f , the parametric curve representing the set of values of function $g(\varepsilon, f)$ has a

countable number of the touch points of loops in the complex plane, while the curve corresponding to the vector function $(g(\varepsilon, f_1), \dots, g(\varepsilon, f_{N_{\text{exp}}}))$ for a selected set of frequencies $(f_1, \dots, f_{N_{\text{exp}}})$ in a multidimensional complex space is not self-intersecting if N_{exp} is large enough. For that reason when switching from a single-frequency to a multi-frequency experiment with a sufficiently small frequency step, Problem 1 of reconstructing the layer real permittivity becomes correct.

4 Multi-frequency Least Squares Method

Problem 3 (least squares method, LSM). Find a real value $\varepsilon^{(\text{layer})}$ satisfying the condition

$$\begin{aligned} & \|g(\varepsilon^{(\text{layer})}, \mathbf{f}) - \mathbf{g}^{\text{exp}}\|_{C^{N_{\text{exp}}}} = \\ & = \min \left(\|g(\varepsilon, \mathbf{f}) - \mathbf{g}^{\text{exp}}\|_{C^{N_{\text{exp}}}}, \varepsilon \in \Omega^{(\varepsilon)} \right) \end{aligned}$$

for a given complex vector $\mathbf{g}^{\text{exp}} \in G(\mathbf{f}, \Omega^{(\varepsilon)})$ with the selected frequency vector $\mathbf{f}$.

Problem 4 (LSM for $N_{\text{exp}} = 1$). Find a real value $\varepsilon^{(\text{layer})}$ satisfying the condition

$$|g(\varepsilon^{(\text{layer})}, f) - g^{\text{exp}}| = \min \left(|g(\varepsilon, f) - g^{\text{exp}}|, \varepsilon \in \Omega^{(\varepsilon)} \right)$$

for a given complex value $g^{\text{exp}} \in G(f, \Omega^{(\varepsilon)})$ with the selected frequency value f .

Figure 4. The branches of the curve $G(f, \Omega^{(\varepsilon)})$, $N_{\text{exp}} = 1$, $f = 9.25 \text{ GHz}$, $\Omega^{(\varepsilon)} = (2.05, 2.08) \cup (3.09, 3.12)$, with the intersection point $g(\varepsilon_1, f) = g(\varepsilon_2, f)$;

● experimental values $\{g_k^{\text{exp}}\}$, ●, ■ $\{g(\varepsilon_k^{(\text{layer})}, f)\}$, $\{\varepsilon_k^{(\text{layer})}\}$ are unstable solution of Problem 4, $k = 1, \dots$

Problems 3 and 4 are solvable [5]; however, when N_{exp} is

a small number the solution can be unstable in the neighborhood of self-intersection points. Figure 4 demonstrates the situation when the solution to Problem 4 differs significantly while the experimental data are close. This obstacle becomes urgent if the domain of location of the sought permittivity admits only a rough estimate and consequently the number and position of self-intersection of the curve generally cannot be predicted. When the number of measurements N_{exp} is large enough, the (unique) solution to Problem 3 exists and depends continuously on possibly inaccurate experimental data; that is, LSM is stable.

In [5] the estimates are obtained of the condition number which shows how much the sought permittivity value can change with a small error in experimental data. The estimates take into account the effect of the size of the layer, width of the frequency band, and its distance to the lowest possible value (cutoff frequency). Applying these results one can get the necessary rate of convergence of the approximate solution to the exact value when improving the quality of experimental data.

Note that a consequence of the proposition is an estimate

$$h^{(f)} \leq h_E^{(f)} = (f_2 - f_1) / N_E$$

for the step of the frequency grid, it is a sufficient condition for the correctness of inverse Problem 1 of determining the layer permittivity in a rectangular waveguide from the data of a perfect (noiseless) multi-frequency experiment and can be used in its planning.

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