Dielectric constant determination of liquid using rectangular waveguide structure combined with EM simulation

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Abstract

The present study aims to contribute for the establishment and validation of numerical simulation of electromagnetic materials complex permittivity using a rectangular wave guide structure. For this purpose, the simulated values of complex permittivity for number of liquids have been determined in the X and Ku bands using software Ansoft HFSS simulator. The simulated results are discussed and compared with results of the literature and the calculated data using theoretical Debye's model. Finally, the percentages of errors between the simulated and theoretical results are estimated. The comparison shows a good convergence, which guarantees the application of the adopted methodologies for the dielectric behavior prediction of different liquid materials in the frequency range [8,2 – 18] GHz.

Keywords: Complex permittivity; Anasoft HFSS Simulator; Waveguide; X and Ku bands.

1. Introduction

The material characterization is an important issue in many material production, processing, management applications in agriculture, food engineering, medical treatments, and bioengineering [1]. The determination of the dielectric properties of liquids has high practical potential in many industrial, medical, as well as environmental sectors [2]. A broad variety of measurement techniques has been proposed in the literature [3]. For the determination of the dielectric properties of liquids, there is several methods available, such as the free-space technique, coaxial probe, waveguide, resonant cavity, and parallel plate [4]. Generally, the choice of a method depends on the kind of material and characterization [5]. Because waveguide measurements are highly sensitive, sample holder preparation is relatively easy and mechanical connections of waveguide sections are simple and robust, waveguide sample holders have effectively been applied for precise and accurate dielectric characterization of liquid samples [6, 7].To obtain the precise permittivity of a liquid sample, we use the rectangular-waveguide transmission line technique for the simulation. In this technique, the sample of liquid is filled in the cross section of the transmission line [6, 8]. The reflection from and the transmission through the sample are measured [9]. The present paper branches out into two related topics. The first one re-examines the Debye mathematical model to retrieve the relative complex permittivity of liquid samples. The second topic is concerned about the implementation of a computational modeling to predict the behavior of electromagnetic materials in confined environment by using electromagnetic three-dimensional simulation Software Ansoft HFSS.

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2. Analysis

Figure 1 shows the waveguide filled with a dielectric sample, where Z_0, γ_0, Z_s, and γ_s are the wave impedance and propagation constant in an air filled and sample filled waveguide, respectively:
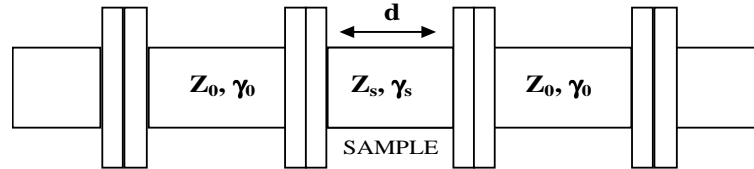

Figure 1 Waveguide filled with single dielectric sample

By the transmission/reflection line theory, the expressions for the total transmission and reflection through a series of dielectric inside a waveguide are given in (1) and (2), respectively. In the analysis, we also assume that the dominant mode TE_{10} is present inside the waveguide [6, 10]:

$$S_{21} = \frac{T_s(1-\Gamma_s^2)}{1-\Gamma_s^2 T_s^2} = \frac{4\gamma_s\gamma_0}{(\gamma_s+\gamma_0)^2 \exp(\gamma_s d) - (\gamma_s-\gamma_0)^2 \exp(-\gamma_s d)} \qquad (1)$$

$$S_{11} = \frac{\Gamma_s(1-T_s^2)}{1-\Gamma_s^2 T_s^2} = \frac{(\gamma_0^2-\gamma_s^2)2\exp(\gamma_s d) - (\gamma_0^2-\gamma_s^2)\exp(-\gamma_s d)}{(\gamma_s+\gamma_0)^2 \exp(\gamma_s d) - (\gamma_s-\gamma_0)^2 \exp(-\gamma_s d)}. \qquad (2)$$

Ts, Γs and d are the transmission coefficient and the reflection coefficient respectively, and d is the sample length.

Where:

$$\gamma_0 = j\beta_0 \qquad (3)$$

$$\gamma_s = \alpha_s + j\beta_s. \qquad (4)$$

The propagation coefficient of an air-filled waveguide is:

$$\beta_0 = \frac{2\pi}{\lambda_0}\left[1-(\frac{\lambda_0}{\lambda_c})^2\right]^{1/2} \qquad (5)$$

The propagation coefficient of a loaded waveguide is:

$$\beta_s = \frac{2\pi}{\lambda_0}\left[(\frac{\lambda_0}{\lambda_c})^2 - \varepsilon_r\right]^{1/2} \qquad (6)$$

λ_0 and λ_c are the wavelength of free space and the cutoff wavelength of the waveguide for TE_{10} mode, and $\varepsilon_r = \varepsilon' - j\varepsilon''$ is the relative complex dielectric constant. It is obvious that S_{11} and S_{21} are functions of complex permittivity of the sample under test. Therefore, once the measured reflection and transmission coefficients are obtained, complex permittivity of the sample can be extracted by an optimization procedure such as the Newton–Raphson method [3], [11]. The equation to solve can be written as follows [12]:

$$\frac{1}{2}\left[(S_{12}+S_{21})+\beta(S_{22}+S_{11})\right] = \frac{T.(1-\Gamma^2)+\beta\Gamma(1-T^2)}{(1-T^2\Gamma^2)} \qquad (7)$$

According to the equation (7), β varies as function of the sample length, uncertainty in scattering parameters, and loss characteristics of material [12]. In the case of a low loss dielectric materials (β=0) and therefore the estimated value is optimal and the complex permittivity is only extracted from the S_{21} parameter [6]. However, only complex permittivities of low-loss liquids were estimated in this work. Theoretically, the well-known Debye's equation is used to carry out the computation of complex permittivity of materials as follows [6]:

$$\varepsilon = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + j.\omega\tau} \qquad (8)$$

ε is the complex permittivity, ε_s is the static permittivity, ε_∞ is the permittivity at the infinite frequency, and τ is the relaxation time. The Debye's parameters of tested liquids from various researchers are shown in table 1. Those parameters were used to calculate the complex permittivity at each frequency over X and Ku bands.

Table 1 Debye's Parameters Obtained from Various Literatures

Material	ε_s	ε_∞	τ (pSec)	Reference
Chlorobenzene	5.54	2.3	10.3	[13]
Butanol	17.1	3	438	[14]
2-Propanol	20.8	3.8	254	[15]
Acetone	21.2	1.9	3.34	[14]

3. Numerical Simulations

A new approach is presented that relies upon 3D electromagnetic simulation results to characterize the complex permittivity of homogeneous low-loss dielectric liquid materials. The numerical simulations were carried out according to flowchart presented in figure. 2. In this case, the relative complex permittivity's of each liquid sample were deduced from a scattering matrix defined between the sample planes. The theoretical constitutive parameters using Debye Model were used in simulation technique to predict the scattering parameters of sample which is completely filled in waveguide.
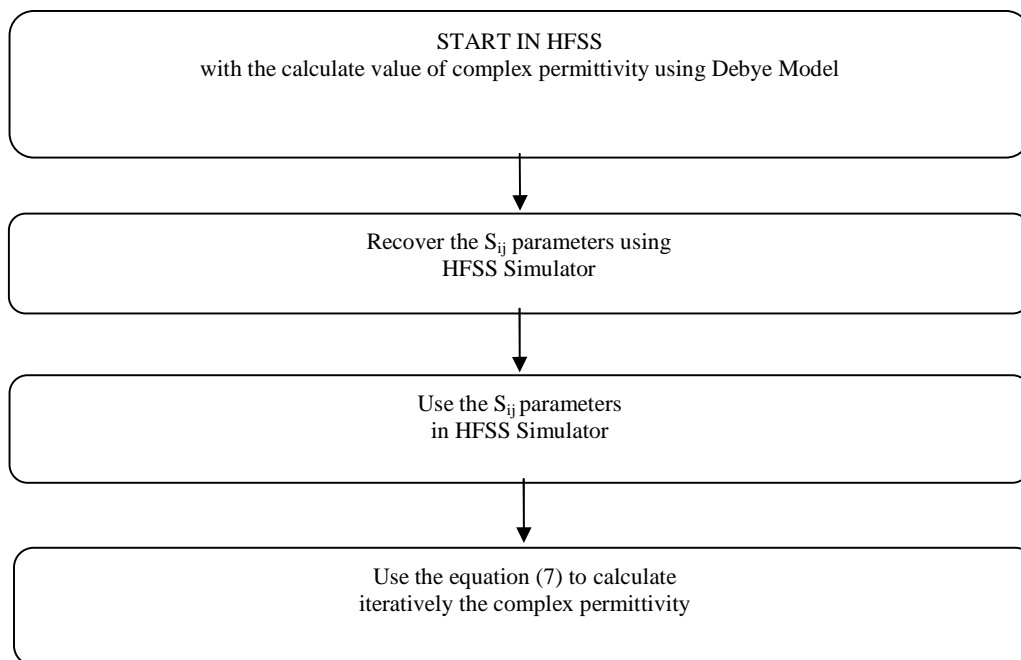
START IN HFSS
with the calculate value of complex permittivity using Debye Model

Recover the S_{ij} parameters using
HFSS Simulator

Use the S_{ij} parameters
in HFSS Simulator

Use the equation (7) to calculate
iteratively the complex permittivity

Figure 2. Flowchart of the numerical simulation used in the complex
permittivity calculation

The iterations continue until convergence which is reasonably quick. Initial estimates can be obtained using Debye's approximations at the starting frequency, with subsequent iterations using the values determined at the previous frequency. A Matlab program was written to obtain relative complex permittivity of sample for 201 frequency points over each band.

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4. Results and Discussion

The procedure has been tested with WR90 and WR62 waveguides operating in the frequency range X and Ku bands respectively. The scattering parameters of the tested structure were obtained by performing simulations using the 3-D electromagnetic software Ansoft HFSS, as this procedure provides flexibility to explore different materials without the need for fabrication [16]. In this approach, we simulated the frequency response of the rectangular waveguide structure by providing specific material characteristics and extracted these parameters from the full-wave EM scattering parameters using the procedure described earlier in figure 2. The design structure in HFSS is presented in figure 3.
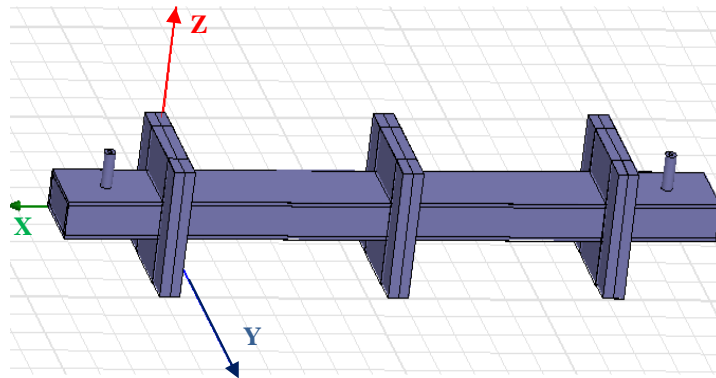

Figure 3. Rectangular waveguide structure simulated using Software Ansoft HFSS

The simulated results of relative complex permittivity of low loss liquid dielectrics, such as Chlorobenzene, Butanol, 2- Propanol, and Acetone are presented in figures 4 – 7, respectively. In order to verify the accuracy of the simulations, all simulated results of each sample are compared to the Debye's equation.
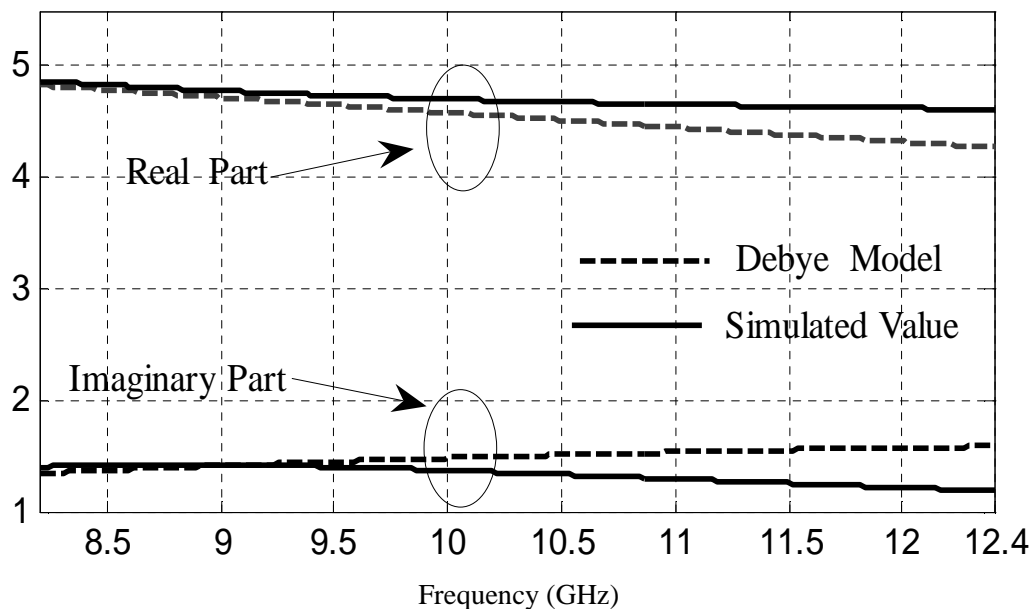

Figure 4-a Simulated and theoretical values of the complex permittivity
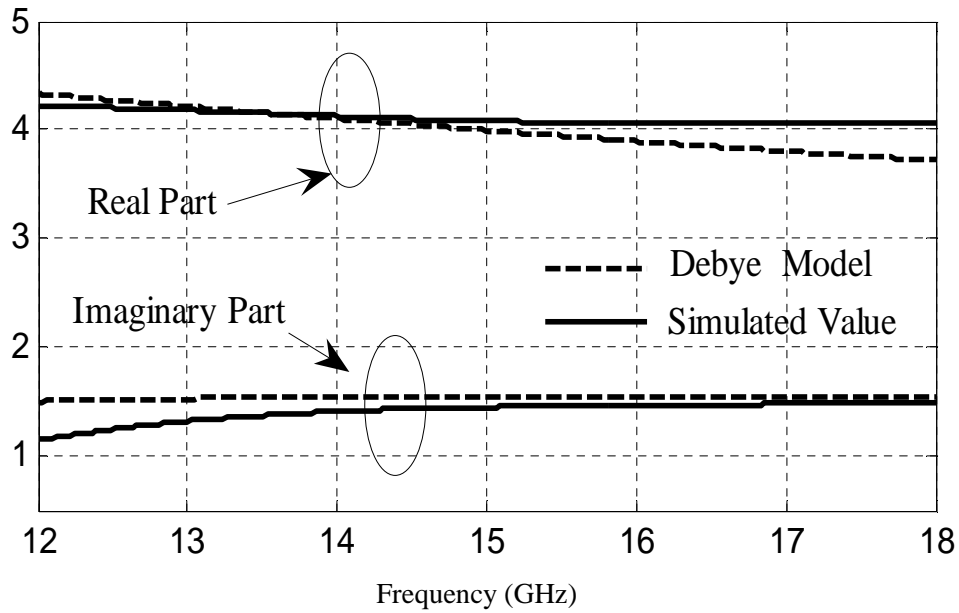of Chlorobenzene sample over the X band

Figure 4-b Simulated and theoretical values of the complex permittivity
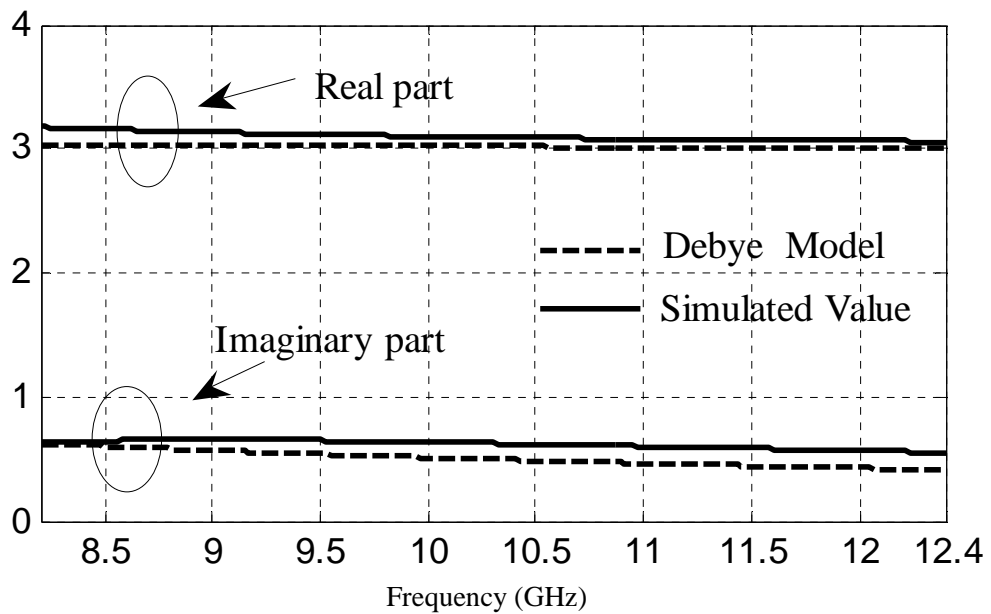of Chlorobenzene sample over the Ku band

Figure 5-a Simulated and theoretical values of the complex permittivity
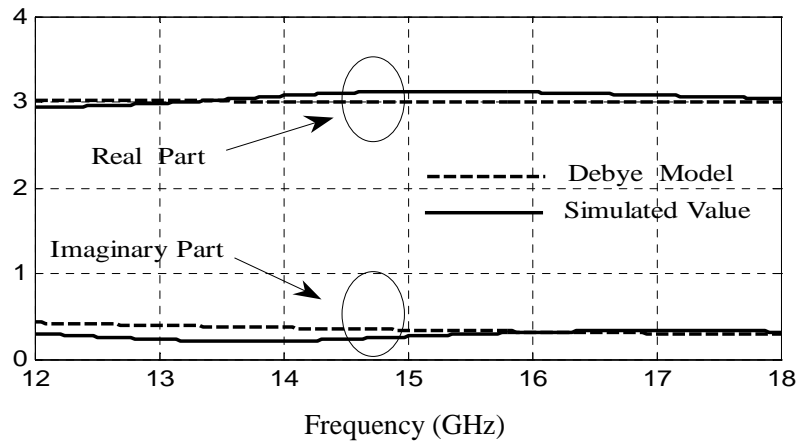of Butanol sample over the X band

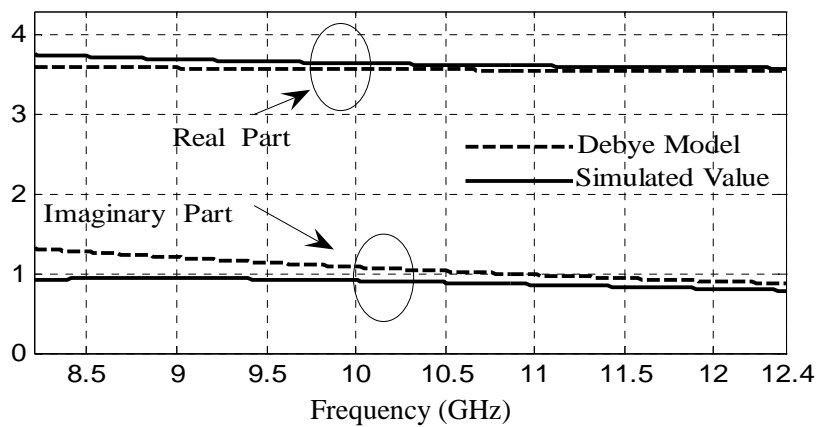**Figure 5-b** Simulated and theoretical values of the complex permittivity of Butanol sample over the Ku band

Figure 6-a Simulated and theoretical values of the complex permittivity of 2-Propanol sample over the X band
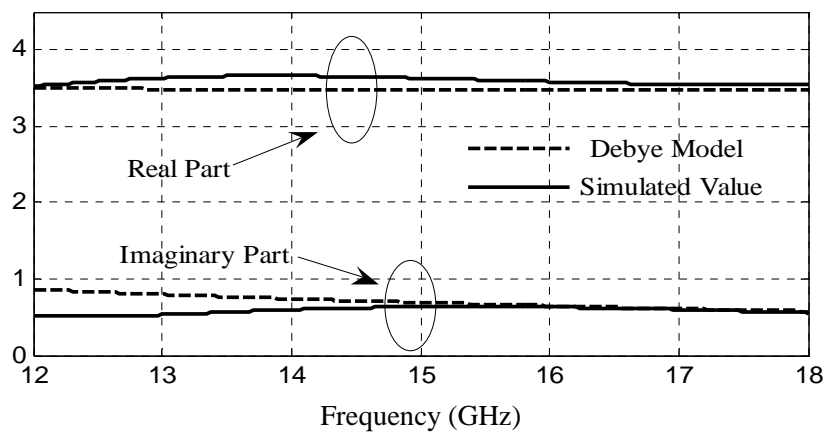

Figure 6-b Simulated and theoretical values of the complex permittivity of 2-Propanol sample over the Ku band
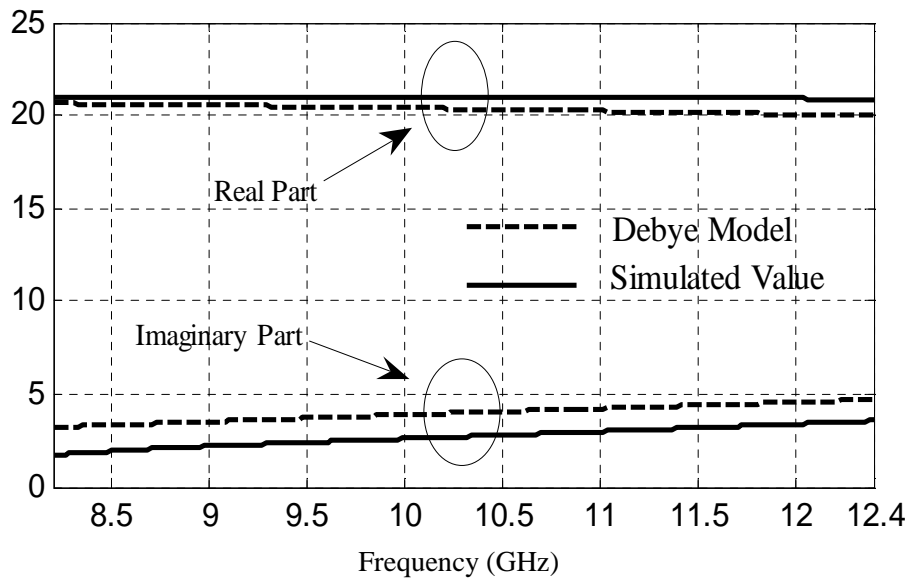
Figure 7-a Simulated and theoretical values of the complex permittivity
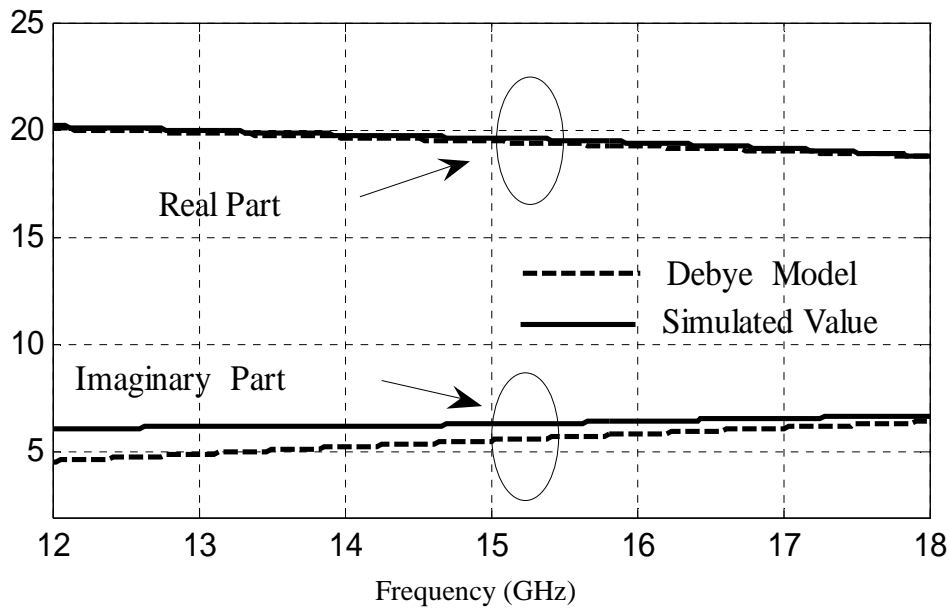of acetone sample over the X band

Figure 7-b Simulated and theoretical values of the complex permittivity
of acetone sample over the Ku band

The simulated values of relative complex permittivity over X and Ku bands of Chlorobenzene, Butanol, 2-Propanol, and Acetone are respectively presented in figures 4 to 7. These results are compared with the theoretical values from the Debye's equation. According to the comparisons, the simulation results show a good agreement. Additionally, it is seen that the simulated values agree reasonably well with the published data [4], [6], [8]. In tables 2 and 3, we show the dielectric constants for selected frequency points across the frequency range from 8.2 through 18 GHz.

Table 2 Dielectric constants for selected frequency points across the X band

Frequency (GHz)	Chlorobenzene		Butanol		2- Propanol		Acetone	
	Simulated value	Debye Model	Simulated value	Debye Model	Simulated value	Debye Model	Simulated value	Debye Model
	ε'	ε'	ε'	ε'	ε'	ε'	ε'	ε'
8.2	4.86	4.86	3.17	3.027	3.75	3.6	20.98	20.64
9.6	4.72	4.68	3.11	3.02	3.65	3.57	21.03	20.44
11	4.65	4.58	3.07	3.01	3.6	3.55	21	20.22
12.4	4.58	4.37	3.05	3.01	3.58	3.53	20.85	19.97

Table 3 Dielectric constants for selected frequency points across the Ku band

Frequency (GHz)	Chlorobenzene		Butanol		2- Propanol		Acetone	
	Simulated value	Debye Model	Simulated value	Debye Model	Simulated value	Debye Model	Simulated value	Debye Model
	ε'	ε'	ε'	ε'	ε'	ε'	ε'	ε'
13.8	4.21	4.21	3.053	3.009	3.66	3.533	19.80	19.7
15.2	4.15	4.07	3.12	3.008	3.62	3.52	19.58	19.41
16.6	4.12	3. 94	3.093	3.006	3.56	3.52	19.24	19.08
18	4.11	3.87	3.04	3.005	3.53	3.51	18.77	18.79

For error estimations, several factors which affect the accuracy of the complex permittivity determination are extensively treated in the literature [12], [17]. In simulation configuration, the sample length and the sample holder length, the reference planes, and uncertainty in magnitude and phase of S_{ij} parameters are accurately known. In this case, we are interested in the percentage error between theoretical values of complex permittivity and those obtained from simulations. The simulated values and theoretical results from Debye's equation are used to find the percentage error of dielectric constant from the following equation:

$$\% \ \text{Error} \ = \frac{\left|\varepsilon'_s - \varepsilon'_d\right|}{\varepsilon'_s} \times 100 \tag{9}$$

Where ε'_s is the dielectric constant from simulations, ε'_d is the dielectric constant using Debye's approximation. The percentage errors of simulated dielectric constant are presented in the histograms (figures. 8 – 9), showing the percentage errors of each tested liquid at selected frequency over X and Ku bands.

It's seen from the histograms that the percentage errors on dielectric constant is between 0 % and 4,8 % on the selected frequency points over the X band. Additionally, the percentage errors are less than 4,2 % on Ku band with the exception of Chlorobenzene where the percentage errors achieve 6,2 % at 18 GHz. In general way, the simulations and Debye model describe pratically the same dielectric behavior of tested liquids. A slight difference between our results and the published values or calculated from Debye's equation can be observed.To understand this difference, it is important to mention that the simulation configuration takes place in an ideal environment, where temperature effect, container effect, evaporation and oxidation leading to the decrease in volume and thickness of liquids in a sample holder, and air gap effects are not taken into account.
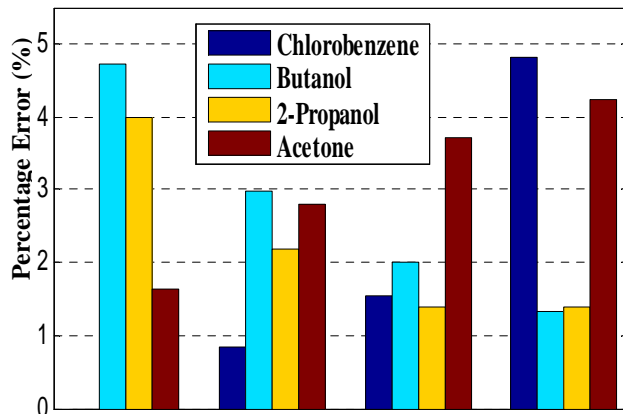
Figure 8 Histograms of the (%) error between simulated and theoretical dielectric constant for Chlorobenzene, Butanol, 2-Propanol, and Acetone for selected frequency points across X band
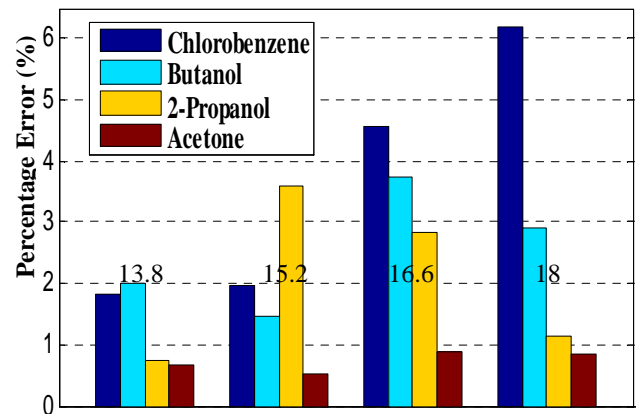
Figure 9 Histograms of the (%) error between simulated and theoretical dielectric constant for Chlorobenzene, Butanol, 2-Propanol, and Acetone for selected frequency points across Ku band

Conclusion

A simulation procedure of rectangular wave guide structure for the determination of complex permittivity of liquid materials has been proposed. The method is based on simulating the S_{ij} parameters of each sample using electromagnetic three-dimensional simulation Software Ansoft HFSS. The simulated parameters are then used to estimate the complex permittivity from a classical Newton-Raphson's method. We have validated the proposed approach with the complex permittivity determination of four liquids in the X and Ku bands. The extracted material parameters are accurate within 6,2 % error for dielectric constant, when compared with the specified values over the frequency range 8,2 – 18 GHz. Considering the simplicity and accuracy over a broad frequency band, this method proves to be useful for the prediction of complex permittivity of liquid materials for a wide range of applications.

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