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Computation of Dielectric Constant and Loss Factor of Water and Dimethylsulphoxide from 0.1 to 13 GHz

Onimisi M.Y.*

Department of Physics, Nigerian Defence Academy, Kaduna, Nigeria

Ikyumbur J.T.

Department of Physics, Federal College of Education, Pankshin, Plateau State, Nigeria

Abstract: This study examined the computation of the dielectric constant (ϵ') and dielectric loss factor (ϵ'') of water and dimethylsulphoxide (DMSO) at temperature 20°C, 30°C, 40°C and 50°C within the frequency range of $0.1 \leq f \leq 13$ GHz using Debye equations. The Debye equations were derived, and the experimental values of the static dielectric constant (ϵ_s), dielectric constant at high frequency (ϵ_∞) and the relaxation time (τ) of water and DMSO at those temperatures were substituted into the derived equations and the dielectric constant (ϵ') and loss factor (ϵ'') of water and DMSO were computed with aid of maple-13 and results were generated. These results revealed that the method is capable of reproducing good results for work done using single Debye and that of the reflection cell of dimethylsulphoxide.

Keywords: Computation; Dielectric constant; Loss factor; Water; Dimethylsulphoxide.

1. Introduction

Dielectric relaxation spectroscopy is a powerful tool for examining the underlying physics of solvent systems [1, 2] and for exploring the molecular dynamics of liquids, which are characterized by inter- and intramolecular structures that vary rapidly with time. Historically, such studies have focused separately on long-range and short-range molecular forces [3]. At one extreme, long-range, nonspecific dispersion forces produce weakly bonded van der Waals complexes, while at the other, short-range, highly directional hydrogen bonding generates molecular networks. In reactions, where the solvent is directly involved in the process (as in solvolytic reactions), the reaction rate can be markedly sensitive to the solvent structure and dynamics [4]. In chemical processing applications, the availability of quantitative data on dielectric properties of solvent systems or methods for their prediction is essential for the design and implementation of microwave heated processes.

Water is one of the most common and most important substances on the Earth's surface. It is essential for the existence of life, and the kinds and amounts of vegetation occurring on various part of the earth's surface depend more on the quantity of water available than any other single environmental factor. Water is the most abundant compound on earth's surface, covering about 70% of the planet [5, 6]. Concerning the structure of water, Smith et al [7] added that the bond between each hydrogen atom and the oxygen atom results from a pair of electrons shared between the hydrogen and oxygen atoms. In water, the electrons in the shared pair are not shared equally between the hydrogen and oxygen atoms. Debye relaxation is generally limited to weak solutions of polar liquids in non-polar solvents. Water in liquid state comes closest to exhibiting Debye relaxation and its dielectric properties are interesting because it has a simple molecular structure. One fascinating thing about water is that it occurs naturally and without it life is not sustained.

The dielectric relaxation of water and DMSO at various temperatures and frequencies has been studied by several authors. Popular among them is complex permittivity of water at 25°C [8], the dielectric relaxation in water in the neighborhood of 4°C [9], complex permittivity of water as a function of frequency and temperature [10] and the dielectric relaxation of water between 0°C and 35°C [11]. Markarian and Stockhausen [12] had studied the dielectric relaxation of Dimethylsulphoxide at 20°C and complex permittivity of dielectric reference liquids including Dimethylsuloxide at frequencies up to 5GHz has been studied by Gregory and Clarke [13]. At microwave and millimetre-wave frequencies, the complex permittivity data can be fitted to the single- Debye equation (3 parameters). This single- Debye equation has used to fit the complex permittivity data of the DMSO by Gregory and Clarke [13] and their measurements was done using coaxial cells (Reflection cells). In this work, we attempt to compute the dielectric constant and loss factor of water and DMSO at temperature between 20°C to 50°C and frequency range of $0.1 \leq f \leq 13$ using Frohlich approach.

The Debye equation that describes a dielectric response with a single relaxation time constant is:

$$(\epsilon' - j\epsilon'') = 1 + \left[\epsilon_\infty - 1 + \frac{(\epsilon_s - \epsilon_\infty)}{(1 + j\omega\tau)} \right] \quad (1)$$

Where ϵ_∞ is the complex permittivity, ϵ_s is the static permittivity and τ is relaxation time. From equation (1), according to Frohlich one can derive both the dielectric constant ϵ' (real part) and loss factor ϵ'' (imaginary part) as shown in equations (2) and (3) below. The detail of mathematical derivation of the dielectric constant ϵ' and loss factor ϵ'' is shown in our other paper [14]. In this paper, we shall derive the mathematical form of the relaxation time.

$$\epsilon' = \epsilon_\infty + \frac{(\epsilon_s - \epsilon_\infty)}{(1 + \omega^2 \tau^2)} \quad (2)$$

The loss factor can be obtained from the imaginary part of equation (1), i.e.

$$\epsilon'' = \frac{(\epsilon_s - \epsilon_\infty) \omega \tau}{(1 + \omega^2 \tau^2)} \quad (3)$$

2. Mathematical Derivation of Relaxation Time, τ

According to Agilent Basics of Measuring the Dielectric properties of materials [15], a material that has a single relaxation frequency as exhibited by the Debye relation will appear as a semicircle with its centre lying on the horizontal $\epsilon'' = 0$ axis and the peak of the loss factor occurring at $\frac{1}{\tau}$.

We recall equation (3), i.e.

$$\epsilon'' = \frac{(\epsilon_s - \epsilon_\infty) \omega \tau}{(1 + \omega^2 \tau^2)} \quad (4)$$

Differentiating equation (4) with respect to $\omega \tau$ using quotient rule gives

$$= \frac{(1 + \omega^2 \tau^2)(\epsilon_s - \epsilon_\infty) - (\epsilon_s - \epsilon_\infty) \omega \tau \cdot 2\omega \tau}{(1 + \omega^2 \tau^2)^2}$$

Simplifying the above expression gives

$$\begin{aligned} \frac{d\epsilon''}{d\omega \tau} &= (\epsilon_s - \epsilon_\infty) \left[\frac{1 + \tau^2 \omega^2 - 2\omega^2 \tau^2}{(1 + \omega^2 \tau^2)^2} \right] \\ &= (\epsilon_s - \epsilon_\infty) \frac{(1 - \omega^2 \tau^2)}{(1 + \omega^2 \tau^2)^2} \\ \frac{d\epsilon''}{d\omega \tau} &= \frac{(\epsilon_s - \epsilon_\infty)(1 - \omega^2 \tau^2)}{(1 + \omega^2 \tau^2)^2} \quad (5) \end{aligned}$$

Equating equation (5) to zero yields because if we assumed that the material is lying below the horizontal $\epsilon'' = 0$ axis.

$$\frac{d\epsilon''}{d\omega \tau} = \frac{(\epsilon_s - \epsilon_\infty)(1 - \omega^2 \tau^2)}{(1 + \omega^2 \tau^2)^2} = 0 \quad (6)$$

$$(\epsilon_s - \epsilon_\infty)(1 - \omega^2 \tau^2) = 0 \quad (7)$$

In equation (7), if $(\epsilon_s - \epsilon_\infty) \neq 0$, then

$$(1 - \omega^2 \tau^2) = 0 \quad (8)$$

Solving for $\omega \tau$ in equation (8), we have

$$\omega^2 \tau^2 = 1$$

$$\Rightarrow \omega \tau = 1 \quad (9)$$

Recall

$$\omega = 2\pi f_r \quad (10)$$

Where f_r is the relaxation frequency. Now substituting equation (10) into equation (9) and then solve for τ , we have

$$\begin{aligned} 2\pi f_r \tau &= 1 \\ \tau &= (2\pi f_r)^{-1} \quad (11) \end{aligned}$$

The values of the complex permittivity ϵ_∞ and static permittivity ϵ_s of dimethylsulphoxide used in this work was adapted from National Physical Laboratory Report MAT 23 [13] and that of water were (adapted from Hasted, 1973 in [16]) as shown tables 1 and 2 below. The values ϵ_∞ and ϵ_s were substituted in equations (2) and (3) and results were generated using Maple-13 as shown in the Appendix A below. The results obtained from this work are shown in figure 1-8 below but details of it and how it is compared with work done using single-Debye equation and measurements done using coaxial cells is shown in Appendix B below.

Table-1. Parameters for Dimethylsulphoxide

Temperature	ϵ_s	ϵ_∞
20	47.13	6.802
30	45.86	6.357
40	44.53	5.828
50	43.19	5.410

Source: NPL Report MAT 23 [13]

Table-2. Parameters for Water

Temperature	ϵ_s	ϵ_∞
20	80.20	5.6
30	76.60	5.2
40	73.20	3.9
50	69.90	4.0

Source: Hasted, 1973 in [16]

Figure-1. The graph of permittivity of DMSO at 20°C against the frequency

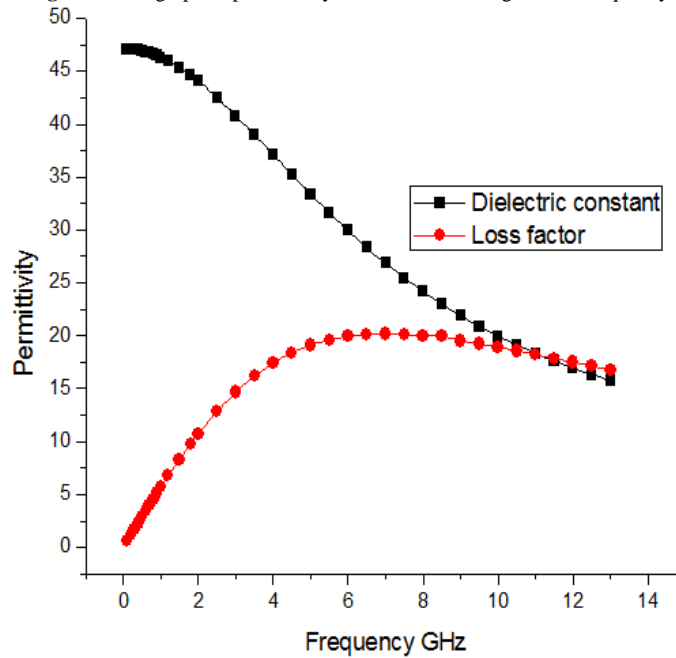


Figure-2. The graph of permittivity of DMSO at 30°C against the frequency

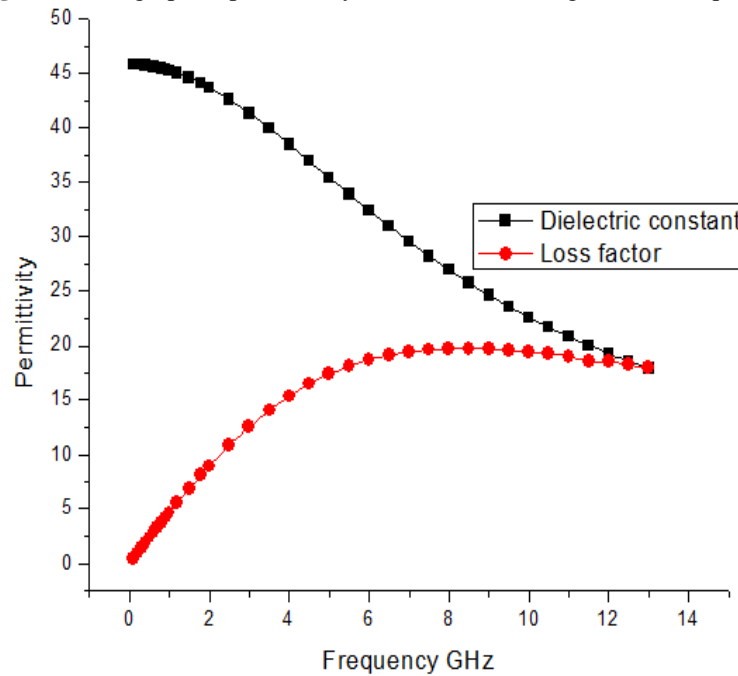


Figure-3. The graph of permittivity of DMSO at 40°C against the frequency

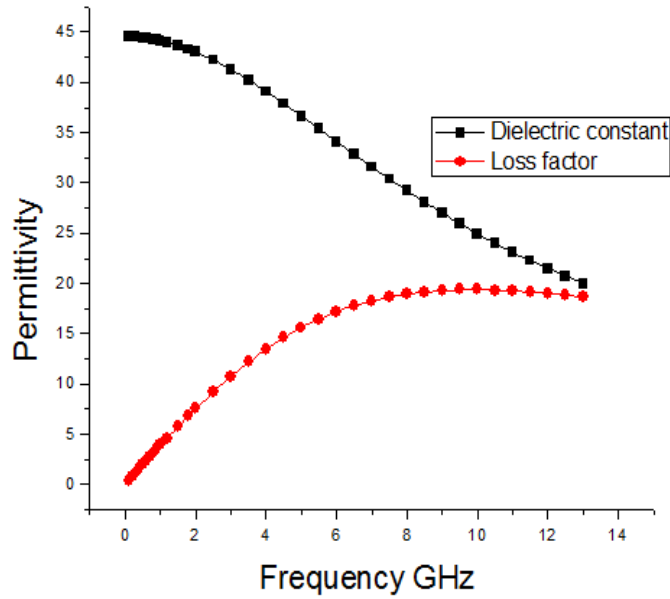


Figure-4. The graph of permittivity of DMSO at 50°C against the frequency

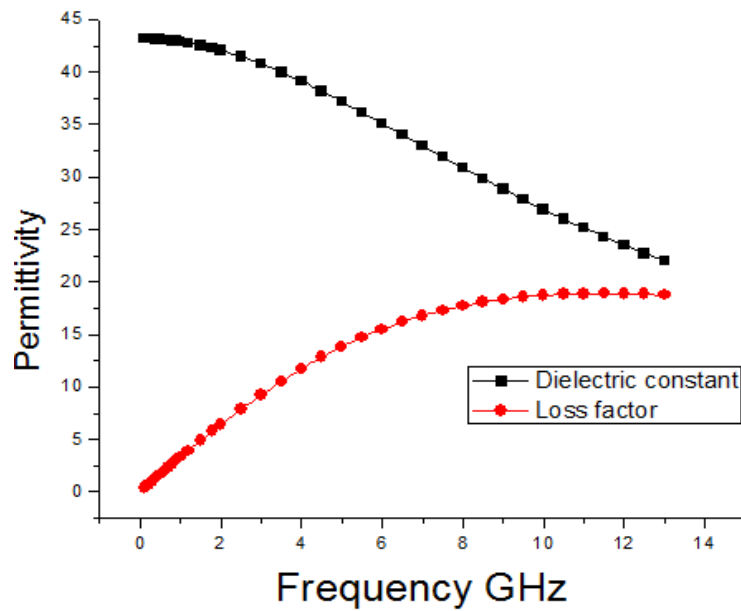


Figure-5. The graph of permittivity of Water at 20°C against the frequency

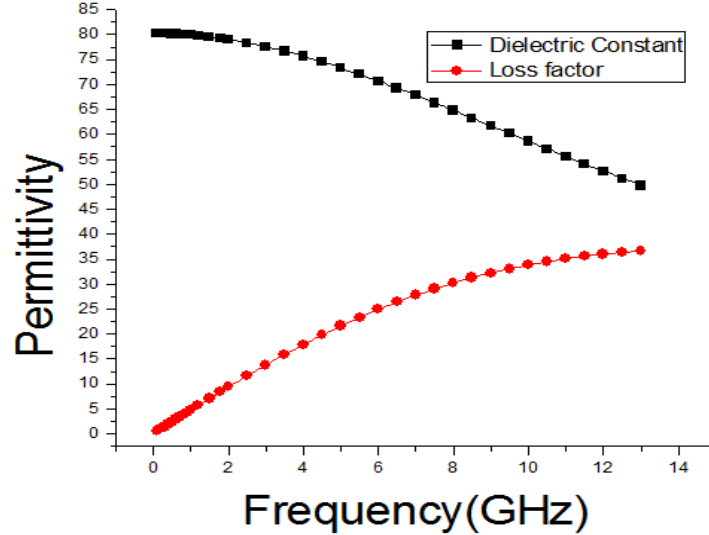


Figure-6. The graph of permittivity of Water at 30°C against the frequency

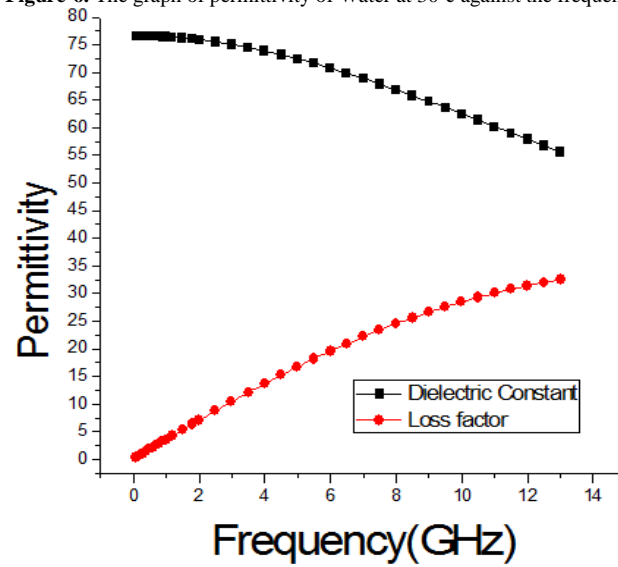


Figure-7. The graph of permittivity of Water at 40°C against the frequency

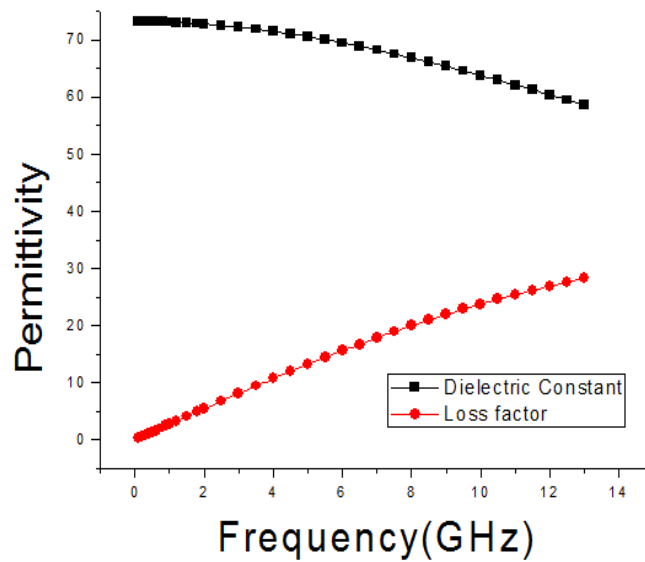
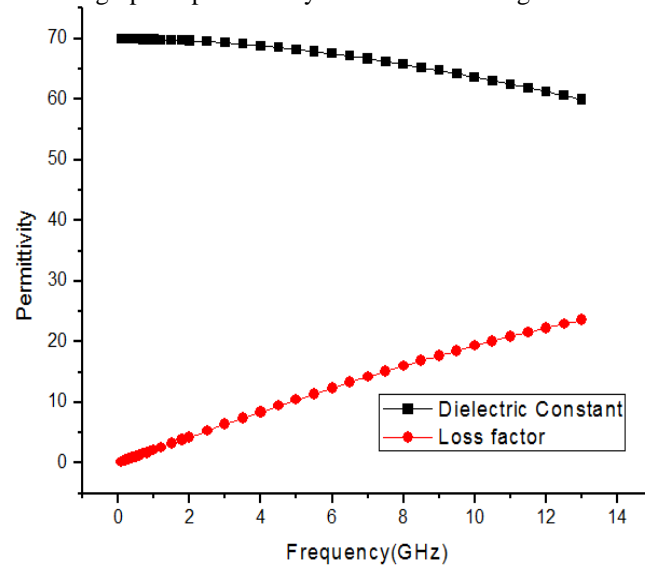


Figure-8. The graph of permittivity of Water at 50°C against the frequency



3. Analysis and Discussion

The dielectric constant and the loss factor of water and dimethylsulphoxide were computed between the frequency ranges $0.1 \leq f \leq 13\text{GHz}$ using Debye relaxation method. The results showed that the dielectric constant ϵ' is higher at low frequencies for both water and DMSO. However, as the temperature increases the dielectric constant for both water and DMSO was found decreasing. But at 10GHz, the dielectric constant was found increasing as the temperature increases from 20°C to 50°C as shown in Appendix B, tables 1-8. This increased in the dielectric constant as observed at frequency 10GHz may be due to the permanent electric dipoles possess by both water and DMSO. The decreased in the dielectric constant as the result of increased in the temperature may be due to the relaxation time which has been found to be fast at high temperatures and decrease dramatically at low temperatures, suggesting a freezing of electric dipoles at low temperatures [17]. The loss factor on the other hand decreases with increase in temperature for both water and DMSO and it was found that the loss factor has its least value at low frequencies as shown in tables 1-8 above.

The higher value of dielectric constant ϵ' at low frequencies may be due to the effect of ionic polarization which varies inversely proportional to the frequency. Water has the highest values of the dielectric constant at all temperatures considered in this work. This implies that water is a better solvent for polar or ionic compounds. The higher value of dielectric constant ϵ' as observed in this work at low frequencies may be because of the overall conductivity which consists of different conduction mechanisms. The most prevalent one in moist materials is the ionic conductivity [18].

The graphs of dielectric constant ϵ' and loss factor ϵ'' against the frequency in gigahertz at various temperatures as shown in figures 1-8 revealed that the dielectric constant ϵ' of both water and DMSO are higher at low frequencies then decreased sharply as the frequency increases and after that it remains almost constant over the entire frequency range. The loss factor ϵ'' which is believed to be dominant by the influence of electrolytic conduction caused by free ions which exist in the presence of a solvent behave very similar in nature like the dielectric constant ϵ' . The loss factor ϵ'' on the other hand decreased rapidly and becomes almost constant afterwards as shown in the above graphs.

The decrease of dielectric constants in higher frequency range for both water and DMSO may be due to the fact that the dipoles cannot follow up the fast variation of the applied field. The higher values of ϵ' and the small values of ϵ'' at lower frequencies may be due to the contribution from all the four types of polarization (i.e. space charge, dipole, ionic and electronic polarization). [19] Observed that at higher frequencies, only the ionic and electronic polarizations contribute. The decrease of dielectric constant ϵ' with increasing frequency means that, the response of the permanent dipoles decreases as the frequency increases and the contribution of the charge carriers (ions) towards the dielectric constant decreases [20, 21].

4. Conclusion

The Debye equation and its derivatives have been used to compute the dielectric constant and loss factor of water and DMSO. The results revealed that within the frequency range of $0.1 \leq f \leq 13\text{GHz}$ and temperature between 20°C to 50°C both water and DMSO obeyed the Debye relaxation method. This showed that the Debye relaxation method and its derivative are capable of mimicking good results for both the coaxial cells and work done using single-Debye.

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