A Numerical Comparision of Dielectric based Measurement of Atmospheric Ice Using Comsol

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Abstract: **A**tmospheric ice is a very complex material with varying electrical properties due to different polymorphs of ice itself. Also, if the medium to be considered is snow, then density becomes an additional parameter because it is a mixture of three dielectrics water, ice and air. The permittivity and loss tangent of naturally occurring ice and snow shows lot of variation at different conditions particularly temperature. This paper is a comparative study of some experimental results found from literature and simulations of dielectric properties of ice and snow in Comsol.

Keywords: Dielectric, Ice, Snow, Conductivity.

1. Introduction

1.1 What is dielectric

A material is defined as 'dielectric' if it has the ability to store energy when it is acted upon by an electrical field. It is directly related with the capacitance. This dielectric constant is also called 'permittivity' which varies with input frequency, surrounding temperature, field and molecular orientation, type of mixture, pressure and molecular structure of material. The dielectric measurements can provide critical design parameter information for many electronic applications.

Following [1] we can define 'C_0' as the capacitance of free space and 'C' as the capacitance of the material then '$C_0=\varepsilon_0 A/t$' and '$C=C_0\varepsilon_r$' where '$\varepsilon_0=8.85\times10^{-12}$ Fm^{-1}', 'A' is the charging surface area and 't' is the distance between the plates. Now if we consider an AC supplied voltage with a frequency 'ω' then across the dielectric material we have a charging current I_C associated with the capacitance and loss current I_L associated with the loss/resistance of the dielectric material (see fig. 1). Hence we can write,

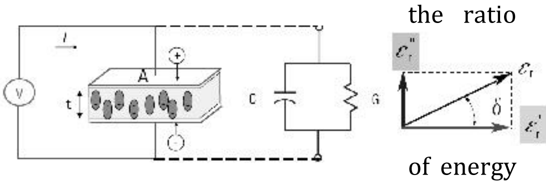
$$I=I_C+I_L=V\left(j\omega C+G\right)=V\left(j\omega C_0\varepsilon_r+G\right) \quad (1)$$

Where 'G' is conductance. Now if we assume $G=\omega C_0\varepsilon''$ then,

$$I = j\omega C_0 V\left(\varepsilon_r' - j\varepsilon_r''\right) = j\omega C_0 V \varepsilon_r \quad (2)$$

Where $\varepsilon_r=\varepsilon_r'-j\varepsilon_r''$ is the complex permittivity which is dependent upon the excitation frequency. Here ε_r' represents the amount of energy from the electric field which is stored in the material and ε_r'' represents how lossy or dissipative a material is to the external electric field. The loss factor includes the effects of both dissipation and conductivity. Also the relative lossiness of the material is the ratio of energy lost to the energy stored and is defined as 'dissipation factor.

$$D = \tan\delta = \varepsilon_r'' / \varepsilon_r' \quad (3)$$



(a) (b)

Figure 1. (a) Dielectric material as a plate capacitor, (b) Argand diagram for dielectric constant

1.2 Water Molecule As A Dielectric Material

A water molecule is a nonlinear polar molecule due to the electronegativity difference of around 1.2 between the constituent elements of H_2O. It has many dielectric mechanisms (atomic, electronic and dipolar) in different frequency domains associated with a cutoff frequency in each domain which appears as a peak in $\varepsilon_r''=\varepsilon_r''(\omega)$ (likewise $D=D(\omega)$) curve. It has strong dipolar effects at low frequencies particularly due to its orientation polarization which are also indicated in the experimental results of [2], [3], [4] and [5]. This dipolar orientation is generally associated with the relaxation[1] phenomenon, whereas the electronic and atomic polarization are associated with the resonance phenomenon. In the frequency domain characteristics the relaxation frequency ‘f_c is indicative of the relaxation time.

2. Mathematical relations and experimental results to be compared/used for determining dielectric properties of ice

Ice as it exhibit dielectric variations can be modeled by the Debye relations which appear in the dielectric response as a function of frequency. In fig. 2 there are some experimental results which reflect the potential of dielectric constant measurements in different frequency spans for ice and snow at different temperatures and different compositions respectively. The Debye relations for pure ice (assumptions are : single relaxation time, zero conductivity and local field same as applied field) are given as,

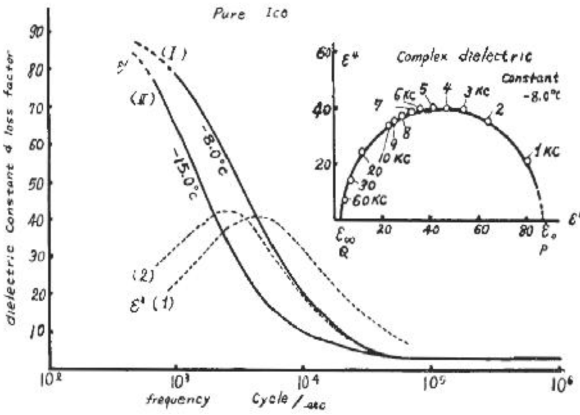
$$
\begin{aligned}
\varepsilon_r^{'} &= \varepsilon_{r\infty} + \frac{\varepsilon_{rs} + \varepsilon_{r\infty}}{1+\omega^2\tau_0^2} \\
\varepsilon_r^{''} &= \frac{\left(\varepsilon_{rs} - \varepsilon_{r\infty}\right)\omega\tau_0}{1+\omega^2\tau_0^2} \qquad (4) \\
\tan\delta &= \frac{\varepsilon_r^{''}}{\varepsilon_r^{'}} = \frac{\left(\varepsilon_{rs} - \varepsilon_{r\infty}\right)\omega\tau_0}{\varepsilon_{rs} + \varepsilon_{r\infty}\omega^2\tau_0^2}
\end{aligned}
$$

Where ε_{rs} is the dielectric constant at zero excitation frequency or dc value, $\varepsilon_{r\infty}$ is the dielectric constant at very high frequency. Few experimental values for ε_{rs}, $\varepsilon_{r\infty}$ and τ_0 for pure ice are given in tab. 1.

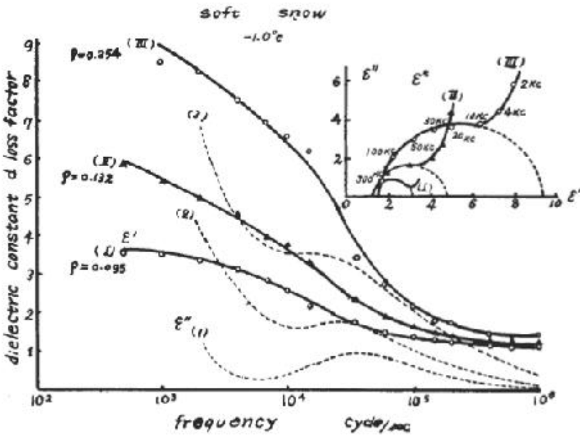
Table 1. Experimental values of ε_{rs}, $\varepsilon_{r\infty}$ and τ_0 [4]

Author	ε_{rs}	$\varepsilon_{r\infty}$	τ_0
Smyth Hiteock	74.60	3.00	$1.846\times10^{-5}\times e^{-0.10158(^{-0}C)}$
Wintsch	73.00	7.50	$2.246\times10^{-5}\times e^{-0.0906(^{-0}C)}$
Errara	77.20	3.00	$2.900\times10^{-5}\times e^{-0.090(^{-0}C)}$
Murphy	95.00	3.50	$1.85\times10^{-5}\times e^{-0.106(^{-0}C)}$

It can be seen from fig. 2a and 2b that there are two different types of plots. The smaller plots are the Argand Diagram which forms a semi circle by sweeping the excitation frequency.



(a)



(b)

Figure 2. (a) Dielectric constant variation as a function of excitation frequency in pure ice at two temperatures (I) and (II) [3]. (b) Dielectric constant variation as a function of excitation frequency for soft snow at (I), (II) and (III) [3].

It is very important to mention that snow is a mixture of three dielectric materials which are air, water and ice. Soft snow is an special case of snow which is a mixture of air and ice only. Hence if the medium being considered is snow then density is also important and this introduces one other parameter which characterizes the shape and orientation of the particles comprising

[1] Relaxation time ‘τ_0’ is a measure of the mobility of the dipoles that exist in the material to reorient themselves.

the mixture. For a mixture of dielectric material we can use the Wiener relation which is given as,

$$\frac{\varepsilon_m - 1}{\varepsilon_m + u} = (\rho)\frac{\varepsilon_1 - 1}{\varepsilon_1 + u} + (1-\rho)\frac{\varepsilon_2 - 1}{\varepsilon_2 + u} \qquad (5)$$

Where 'ε_m' is the dielectric constant of the mixture, 'ε_1' and 'ε_2' are the dielectric constants of two materials and 'ρ' is the proportion of the total volume occupied by medium '1' and u is the Formzahl number, fig. 3. For more details on the dielectric mixing formula reference can be made to tab. 2 in reference [3].

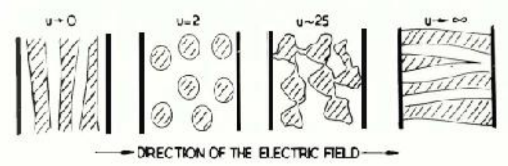


Figure 3. Variation of 'u' with respect to the direction of electric field [4]

Using eq. 5, the following formula is derived when we substitute $\varepsilon_1 = \varepsilon_{ice}$ and $\varepsilon_2 = \varepsilon_{air} = 1$,

$$\varepsilon_d' = \frac{(\rho u - u - \rho u\varepsilon_{ice}' - \varepsilon_{ice}')(\rho\varepsilon_{ice}' - \rho - u - \varepsilon_{ice}') - (\rho\varepsilon_{ice}'' - \varepsilon_{ice}'')(\rho u\varepsilon_{ice}'' + \varepsilon_{ice}'')}{(\rho\varepsilon_{ice}' - \rho - u - \varepsilon_{ice}')^2 + (\rho\varepsilon_{ice}'' + \varepsilon_{ice}'')^2}$$
$$\varepsilon_d'' = \frac{-(\rho u - u - \rho u\varepsilon_{ice}' - \varepsilon_{ice}')(\rho\varepsilon_{ice}'' - \varepsilon_{ice}'') - (\rho\varepsilon_{ice}' - \rho - u - \varepsilon_{ice}')(\rho u\varepsilon_{ice}'' + \varepsilon_{ice}'')}{(\rho\varepsilon_{ice}' - \rho - u - \varepsilon_{ice}')^2 + (\rho\varepsilon_{ice}'' - \varepsilon_{ice}'')^2} \qquad (6)$$

Where ε_d' is the real part and ε_d'' is the complex part of the dielectric constant of dry snow.

In fig. 2b it is clearly visible that at $f<10^4$ there are some deviations in the dielectric constant which are due to the conductivity of H_2O in the snow. These conductivities effects are not dominant in pur ice because the permittivity of pure ice is relatively very larger than that of snow. If the DC conductivity 'σ' is not negligibly small, the σ will also contribute to the imaginary part of the complex dielectric constant [6]. The total dielectric constant will then be mathematically represented as,

$$\varepsilon_r^* = \varepsilon_r' - j\left(\varepsilon_r'' + \frac{\sigma}{\omega}\right) \qquad (10)$$

Therefore by substituting eq. (10) into Debye equation (eq. 4) we get,

$$\varepsilon_r^{*\prime} = \varepsilon_r' = \varepsilon_{r\infty}^* + \frac{\varepsilon_{rs}^* + \varepsilon_{r\infty}^*}{1+\omega^2\tau_0^2}$$
$$\varepsilon_r^{*\prime\prime} = \frac{(\varepsilon_{rs}^* - \varepsilon_{r\infty}^*)\omega\tau_0}{1+\omega^2\tau_0^2} + \frac{\sigma}{\omega\varepsilon_0} \qquad (11)$$
$$\tan\delta^* = \frac{\varepsilon_r^{*\prime\prime}}{\varepsilon_r^{*\prime}} = \frac{\omega\varepsilon_0(\varepsilon_{rs}^* - \varepsilon_{r\infty}^*)\omega\tau_0 + (1+\omega^2\tau_0^2)\sigma}{\omega\varepsilon_0(\varepsilon_{rs}^* + \varepsilon_{r\infty}^*\omega^2\tau_0^2)}$$

This conductivity is a also a function of excitation frequency hence we have followed [7] and used,

$$\sigma(\omega) = \sigma(0) + A\omega^n \qquad (12)$$

Where $\sigma(0)$ and A are assumed to be empirical constants and ω is the excitation frequency. In tab. 2 there are some experimental results found by [8] which are used to compare/assume the conductivity values,

Table 2. Experimental Values Of Direct Current Electrical Conductivities [8]

Material	*Temp.* ^oC	*Cond.* *mho/m*	ε_r	ω*(c/s) for* $\tan\delta = 1$
Pure ice	-10 -40	10^{-7} $3x10^{-9}$	95 105	20 0.5
Soft snow ρ*=0.13 g/cm*^{3}	-10 -40	10^{-9} $3x10^{-11}$	4 4	4 0.1
Granular snow ρ*=0.4 g/cm3*	-10 -40	10^{-7} 10^{-9}	15 15	100 1

In the case of snow, the relaxation time also deviates as all bodies in it are not identical in size, and their orientations involve more than one relaxation time, e.g. if we have ellipsoidal shape of ice molecules, then friction coefficients of the three axes are different, which leads to the existence of three different relaxation times. In this case, a distribution of relaxation times is necessary to interpret the experimental data. Fuoss and Kirkwood [9] have also proposed a parameter λ in the interval [0,1] to take into account the distribution of relaxation times empirically. For λ=1 we have the same Debye equations, hence smaller λ provides large number of relaxation times. Their relation for ε_r'' is given as,

$$\pounds_r^{"} = \frac{a\left(\pounds^*_{rs} - \pounds^*_{r\infty}\right)}{\left(\mu 2_0\right)^{a} + \left(\mu 2_0\right)^{-a}} \qquad (13)$$

Nevertheless the temperature is the most important parameter which directly affect all other parameters. It can be seen in tab. 1 that different researchers have used relations for determining the relaxation time τ_0 for ice. The general relationship that can be formulated and is given as,

$$2 = 2_h e^{\frac{H}{kT}} \qquad (14)$$

Where '2_h' is a pre exponential factor and 'H' is the activation energy, 'T' is the absolute temperature and 'k' is the Boltzmann constant.
It is clearly reflected from fig. 2 that both parts of the complex dielectric constant decrease with increasing temperature and the loss peak shifts towards higher temperatures, as can be seen.

3. Use of Comsol Multiphysics

This software is very versatile as it made the study relatively easy. The 'electrostatics' module was used for this study as the frequencies that we were dealing were relatively small $f<10^7$ Hz.

A simple geometry of a new material 'ice' with varying dielectric properties, dependent on temperature, conductivity and relaxation time was introduced using the equations described in the last section. Similarly another material dry snow was taken into consideration which have an additional parameter of density 'ρ' and wet snow with one another parameter wetness 'W' was taken into consideration. The geometry is kept same for all of the above three materials which is given in fig. 4 (units are in cm). The boundary conditions are defined as the side 3 is such that.

Side 3 = 9 Volts
Side 2 = 0 Volts (Ground)

Free triangular meshing was done to check the application of dielectric equations on this model. A frequency sweep from 0 Hz till 500 MHz, temperature sweep from -1^{0}C till -15^{0}C and density ratio of material 1 and material 2 defined by ρ was swept from 0.1 till 0.9 was used during the simulations.

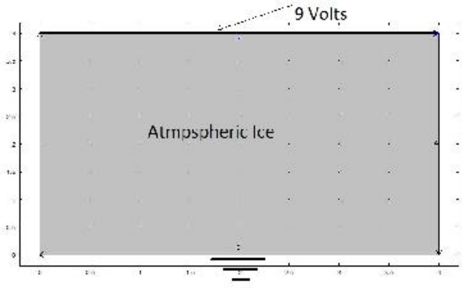


Figure 4. Geometry and boundary conditions of atmospheric ice model.

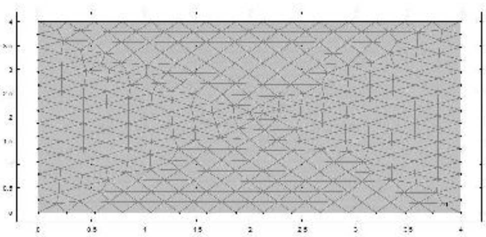


Figure 5. (a) Meshing of the model

4. Comsol Results

The results of Comsol are very impressive as they are quite similar with the experimental results of fig. 2. The argand diagram for pure ice and relative permittivities vs omega at different temperatures are given in fig. 6 and 7 respectively. Also the argand diagram and relative permittivities of dry snow at different density ratios are plotted in fig. 8 and 9.

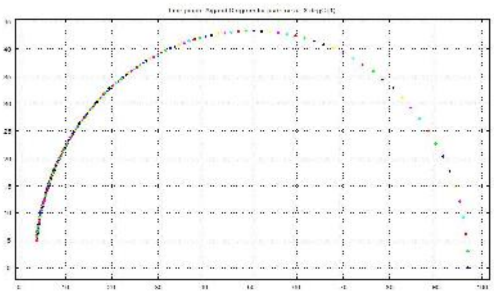


Figure 6. Argand diagram for pure ice at -8^{0}C

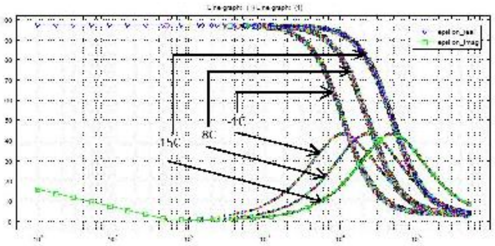


Figure 7. Relative permittivity vs omega at different freezing zones.

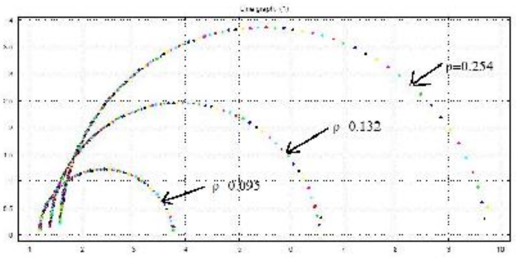


Figure 8. Argand diagram for snow at different density ratios.

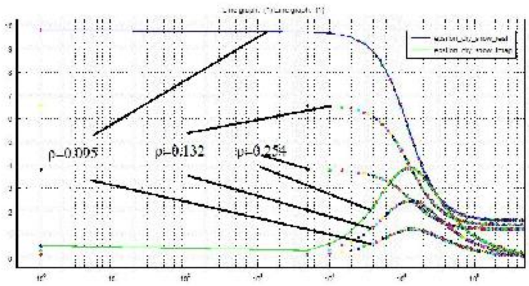


Figure 9. Relative permivities of snow at different density ratios.

5. Conclusions

It is found from this numerical study that Debye equations (eq. 4) forms a basis for the dielectric based sensing technique for atmospheric icing at different temperature. To introduce the variations due to temperature eq. 14 is very useful which is further supported by tab. 1. Also to model snow is little tricky due to the mixture of dielectric materials but the mixing formula eq. 5 is solved to find eq. 6 which is then used to find the variations in the dielectric properties of dry snow at different density ratios. Fig. 6 and 7 is quite similar with fig. 2a and fig. 8 and 9 matches with fig. 2b. Although there are some variations which are due to the conductivity eq. 12 which also depend on temperature but still not validated in these formulations.

6. Future Work

Modeling wet snow is much more difficult then it is understood as it involves three dielectrics water, ice and air. Although some mathematical relations do exist for dry snow but for wet snow even there are not enough mathematical study which can be very interesting to formulate and to justify numerically. Also in this paper conductivity is assumed to be a function of excitation frequency but it is not completely true as it also depends on temperature. Hence to find a conductivity relation as a function of temperature and frequency and then to numerically justify this can also be very interesting.

7. References

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