

MODEL OF DIELECTRIC CONSTANT OF BOUND WATER IN SOIL FOR APPLICATIONS OF MICROWAVE REMOTE SENSING

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Abstract—The paper suggests a model of dielectric properties of bound water in wet soils. The application of the model to the description of dielectric and radiophysical properties of wet soils in microwave electromagnetic range is considered. The comparisons of theoretical and experimental dielectric constants provided show good reliability of the suggested model.

1 Introduction

2 Model of Dielectric Properties of Bound Water in Soil

3 Model of Permittivity of Wet Soils

4 Comparison of Model Calculations and Experimental Data

5 Conclusion

Acknowledgment

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1. INTRODUCTION

Methods of passive microwave sensing of soil can be used to retrieve the type, wetness and wetness profile of a soil, to map ground waters, etc. This information is helpful in the solution of many problems such as river flood forecast, harvest estimations, irrigation planning, meteorological modeling. However, considerable difficulties arise when interpreting data of soil remote sensing. Their origin lies in the

great variety of existing soils (different structural and mineral content) as well as in the complexity of a soil (first of all, the presence of bound and free water and its distribution amongst soil particles). To overcome those difficulties, it is necessary to develop an applicable electrodynamic model of soil taking into account its real physical and structural properties.

At present, many models of wet soil permittivity exist reflecting to greater or smaller extent the real physical and structural picture of soil (see, for example, [1–4]). Those models either do not take into consideration dielectric properties of bound water at all or introduce them artificially (see, for example, [3, 4]). In some cases this leads to a discordance of theoretical and experimental dielectric constants of wet soils. Also, some works [5, 6] attempt to create a physical model of dielectric properties of bound water in soil. However, practical application of that model is rather complicated since analytical calculation of some parameters is impossible and they have to be retrieved experimentally for each type of soil.

From our point of view, modeling of dielectric properties of bound water is hampered by two factors: the great variation of soil water classifications [7] and controversial data on physical properties of water in contact with soil particles [8, 9]. Physical characteristics of bound water are not well enough investigated. For a long time, bound water was considered to have an ice-like structure. The current understanding suggests that the closer the water layer is to the particle the more distorted is its structure compared to the structure of free water and ice [8, 9]. Structure distortion of water close to a surface (soil particles) in comparison to free water brings about changes in its physical properties: density, freezing temperature, dielectric constant, etc. [1, 8–11]. However, existing data on these properties differ greatly [1, 8–11]. As to the classification of soil water, specialists of different fields have different approaches to this problem emphasizing, as a rule, this or that feature of interaction of water with soil skeleton. Generally, modeling of dielectric properties of soil employs water classifications adopted in soil science and geology. According to those classifications, bound water is the water held in soil by electromolecular and molecular surface forces, and free water is the water held solely by gravitation in non-capillary by size macro pores (> 1 mm) and clefts [7, 12]. Soil water classification variations entail different methods of estimation of the amount of bound water in soil when developing soil electrodynamic models [2, 4–6], from one monomolecular layer of water covering soil particles [4] to all non-gravity water in the soil [5, 6].

Therefore, keeping in mind all the above problems related to electrodynamic modeling of wet soils, it is vital, first, to work out

more strict definitions of bound and free water and their volume in wet soils and, second, to develop a practically applicable model of dielectric properties of bound water in soil. These problems are in the focus of the present work.

2. MODEL OF DIELECTRIC PROPERTIES OF BOUND WATER IN SOIL

We believe that when elaborating an electrodynamic model of soil, in order to determine the volume of bound water held in it, one should proceed not from classifications adopted in soil science and geology, but from dielectric properties of water in soils. Here we will consider water bound if its dielectric constant differs from that of free water.

To begin our determination of the volume and dielectric constant of bound water in soil, let us remind the following well-known facts. In [9, 11], it is shown, based on experimental data, that relaxation time τ_{bw} of bound water molecules differs from relaxation times τ_w and τ_i of free water and ice and $\tau_w < \tau_{bw} < \tau_i$. On the other hand, as shown in [9], with the increase of volume of water in clay τ_{bw} approaches τ_w . An analysis [9] of spectra of nuclear magnetic resonance of bound water films in clay give upper limits of relaxation time of bound water molecules at $+27^\circ\text{C}$ depending on the number of monomolecular layers of water covering soil particles. The studies demonstrate that τ_{bw} decreases with the number of monomolecular layers of water covering the particles (see table) and τ_{bw} does not differ from τ_w at film thickness of 10 monomolecular layers.

Number of monomolecular layers of water	Relaxation time of water molecules $\tau_{bw}(+27^\circ\text{C}), s$
1	5.0×10^{-10}
2	5.0×10^{-11}
4	2.2×10^{-11}
10 (free water)	7.7×10^{-12}

Proceeding from the above facts and assuming that bound water dielectric constant as well as that of free water complies with the Debye model, we can state the following:

1. Water in soil remains bound when soil wetness increases from zero to a certain value.

2. Change in volume of bound water in soil leads to the change in its dielectric properties as bound water molecule relaxation time changes.
3. At a certain wetness of soil, dielectric properties of bound water in it become similar to dielectric properties of free water [9]. Further increase of wetness has no impact on soil bound water dielectric constant which remains equal to free water dielectric constant.

Based on τ_{bw} values, obtained in [9] and given in the table, we have defined an approximation of τ_{bw} depending on the thickness h of the film covering soil particles. This dependence has the following form:

$$\tau_{bw}(+27^\circ\text{C}) = \left(-4.9648 \times 10^{24} h^2 - 3.0867 \times 10^{11} \ln(h) - \frac{7.5092 \times 10^3}{h} + 3.9121 \times 10^{18} h - 5.2036 \times 10^{12} \right)^{-1}, \quad (1)$$

where τ_{bw} is in seconds, and h is in centimeters. Formulating this dependence, we assumed that τ_{bw} became equal to τ_w at the water film thickness of 10 diameters of water molecule — h_{10} (water molecule diameter is 2.8×10^{-8} cm [13]). At $h \geq h_{10}$, we assumed $\tau_{bw} = \tau_w$.

Figure 1 presents experimental dependencies of τ_{bw} on the thickness of water film (number of monomolecular layers) covering soil particles as well as a curve approximating these data (1). Mean square deviation of approximated τ_{bw} from experimental data did not exceed 4.2783×10^{-14} sec, maximum deviation was 1.8842×10^{-13} sec.

For bound water dielectric constant ε_{bw} ($\varepsilon_{bw} = \varepsilon'_{bw} + i\varepsilon''_{bw}$), the relaxation model [14] of free water dielectric constant ε_w ($\varepsilon_w = \varepsilon'_w + i\varepsilon''_w$) was used:

$$\begin{aligned} \varepsilon'_w &= \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)}{1 + (\lambda_w/\lambda)^2}, \\ \varepsilon''_w &= \frac{(\varepsilon_s - \varepsilon_\infty)(\lambda_w/\lambda)}{1 + (\lambda_w/\lambda)^2}, \end{aligned} \quad (2)$$

where λ is wavelength, in centimeters, other parameters were retrieved from the following expressions [14]:

$$\begin{aligned} \varepsilon_s(t) &= 87.74 - 0.4008t + 9.398 \times 10^{-4}t^2 + 1.41 \times 10^{-6}t^3, \\ \varepsilon_\infty &= 4.9, \\ \lambda(t) &= 3 \times \left(1.1109 - 3.824 \times 10^{-2}t + 6.938 \times 10^{-4}t^2 - 5.096 \times 10^{-6}t^3 \right), \end{aligned} \quad (3)$$

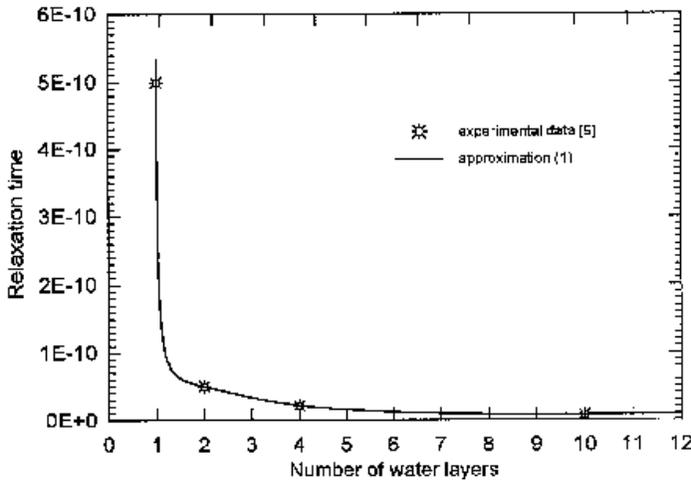


Figure 1. Experimental data and approximation of bound water relaxation time dependence on the number of layers of water covering soil particle.

where t is Celsius temperature of water. The model is distinguished for adequate description of both dielectric constant and relaxation wavelength λ_w of free water [15].

With the relaxation time of bound water at $+27^\circ\text{C}$, known from (1), we can retrieve bound water relaxation wavelength at the same temperature:

$$\lambda_{bw}(+27) = 2\pi c\tau_{bw}(+27), \tag{4}$$

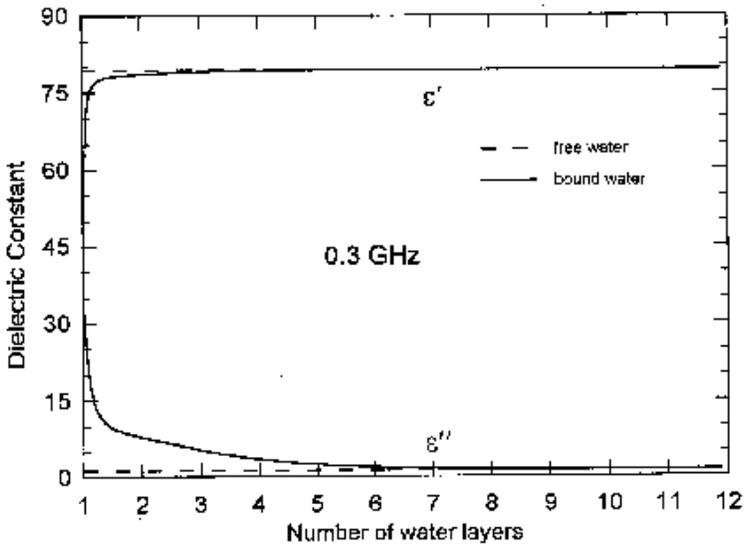
where c is speed of light. Assuming that there are proportional dependencies between $\lambda_{bw}(+27^\circ\text{C})$, $\lambda_w(+27^\circ\text{C})$ and $\lambda_{bw}(t)$, $\lambda_w(t)$, we get:

$$\lambda_{bw}(t) = \lambda_{bw}(+27) \frac{\lambda_w(t)}{\lambda_w(+27)}. \tag{5}$$

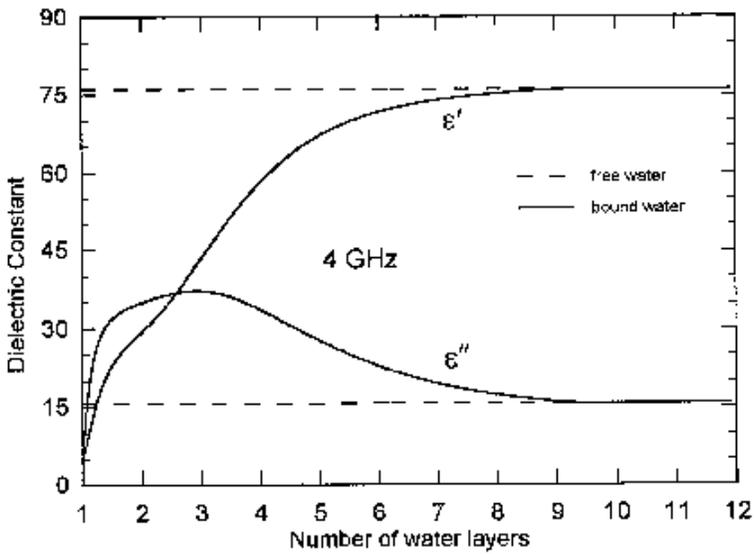
Then, real and imaginary components of bound water dielectric constant can be found from expressions similar to (2), where $\lambda_w(t)$ is substituted by $\lambda_{bw}(t)$ obtained from (5), (4), (3) and (1):

$$\begin{aligned} \epsilon'_{bw} &= \epsilon_\infty + \frac{(\epsilon_s - \epsilon_\infty)}{1 + (\lambda_{bw}(t)/\lambda)^2}, \\ \epsilon''_{bw} &= \frac{(\epsilon_s - \epsilon_\infty)(\lambda_{bw}(t)/\lambda)}{1 + (\lambda_{bw}(t)/\lambda)^2}, \end{aligned} \tag{6}$$

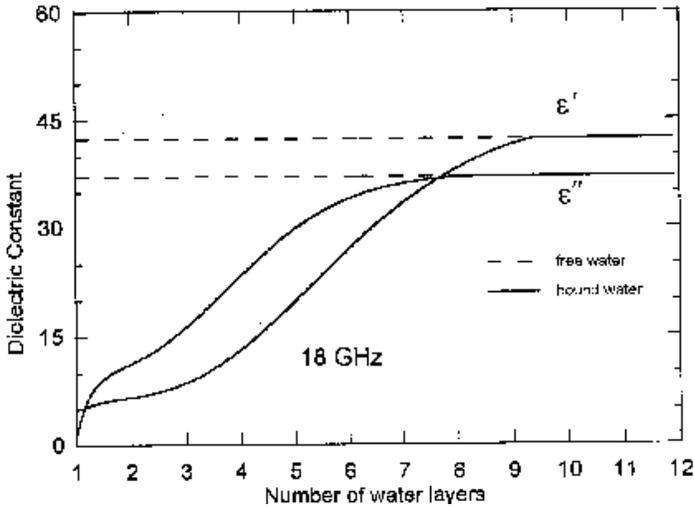
here ϵ_s and ϵ_∞ are defined in the same way as for free water (3).



(a)



(b)



(c)

Figure 2. Real (ϵ') and imaginary (ϵ'') parts of dielectric constant of bound water at sandy loam on number of water layers at frequencies of 0.3 GHz (a), 4 GHz (b), 18 GHz (c). (Dotted line — free water ϵ' and ϵ'').

We have thus determined expressions for the calculation of complex dielectric constant of bound water in soil depending on the thickness of bound water film covering soil particles. The film thickness can be retrieved based on the available soil wetness and modeling approach.

Figure 2 shows dependencies of real and imaginary parts of bound water permittivity on the number of monomolecular layers of water covering soil particles at frequencies of 0.3 GHz (a), 4 GHz (b) and 18 GHz (c), at temperature of +22°C, obtained from (6). It is clear from the figures, that the dependencies of bound water permittivity on the number of monomolecular layers of water covering soil particles vary for different frequencies.

3. MODEL OF PERMITTIVITY OF WET SOILS

Soils are characterized by complex structural and granulometric composition. At present, there is a great variety of granulometric classifications of soils. The most simple and frequently used in radiophysical studies is the classification of USA Department of

Agriculture [2, 4]. According to that classification, the following granulometric fractions are distinguished: sand-particles of diameter $d > 0.005$ cm, silt — 0.0002 cm $< d < 0.005$ cm, clay — $d < 0.0002$ cm, weight content of which is expressed in percentage of total weight of soil. As to stratum composition and dielectric permittivity (in the range 1–50 GHz) of these fractions, it turns out that sand consists primarily of quartz and feldspar with complex dielectric constant $\varepsilon_{sa} \approx 4.5 + i0.05$ [16, 17]; silt — from quartz and muscovit [12] with $\varepsilon_{si} \approx 45 + i0.1$ [16, 17]; clay — from kaolinite and montmorillonite [12], with $\varepsilon_{cl} \approx 4.5 + i0.25$ [16, 17]. Densities of these strata are similar and make 2.5–2.7 g/cm³. It is shown in [2, 13], that the quantity of bound water in soil depends on the volume of clay fraction in it, and the quantity of bound water increases with the volume of clay. This is explained by a large specific area of clay surface compared to other soil fractions.

We will model a wet soil as an aerial medium with spherical inclusions of particles divided into 3 fractions: sand, silt and clay with dielectric constants ε_{sa} , ε_{si} and ε_{cl} , respectively. We will assume that at volumetric wetness V_w growing from 0% to $\max(V_{bw})$, at which bound water dielectric properties become similar to those of free water, water is present only in the shape of films around clay particles and is bound. At wetnesses $V_w \geq \max(V_{bw})$, water in films covers particles of all fractions and is free. In agreement with these views on soil and with [18–20], permittivity of wet soil $\varepsilon_{eff}\varepsilon'_{eff} + i\varepsilon''_{eff}$ can be found from the equation:

$$\varepsilon_{eff}^{-1} = 1 - \frac{4\pi n_{cl} (\varepsilon_{cl}^{bw} + 2) \frac{\langle f_w \rangle_{cl}}{k^2}}{2\varepsilon_{eff} + \varepsilon_{cl}^{bw}} - \frac{4\pi n_{sa} (\varepsilon_{sa}^w + 2) \frac{\langle f_w \rangle_{sa}}{k^2}}{2\varepsilon_{eff} + \varepsilon_{sa}^w} - \frac{4\pi n_{si} (\varepsilon_{si}^w + 2) \frac{\langle f_w \rangle_{si}}{k^2}}{2\varepsilon_{eff} + \varepsilon_{si}^w} - \frac{4\pi n_w (\varepsilon_w + 2) \frac{\langle f_w \rangle_w}{k^2}}{2\varepsilon_{eff} + \varepsilon_w}, \quad (7)$$

where n_{cl} , n_{sa} , n_{si} and n_w are concentrations of clay, sand, silt particles and water drops, respectively; ε_{cl}^{bw} is permittivity of a clay-particle covered by bound water film; ε_{sa}^w and ε_{si}^w are permittivities of sand- and silt-particles covered by bound water film; ε_w is dielectric constant of free water; $\langle f_w \rangle_{cl}$ is averaged over particle sizes amplitude of forward scatter of clay particle covered by bound water film; $\langle f_w \rangle_{sa}$, $\langle f_w \rangle_{si}$ and $\langle f_w \rangle_w$ are averaged over particle sizes amplitudes of forward scatter of sand- and silt-particles covered by free water film and a spherical drop of water, respectively. Scatter amplitudes are calculated according to the Mi theory [21]. Sizes of particles

of many natural media, including soils, conform with the log-normal distribution [12] used for averaging over particle sizes in our model. Effective dielectric constant of soil particles covered by water film, ε_{cl}^{bw} , ε_{sa}^w , ε_{si}^w are defined by the Braggeman formula [21]. The choice of this formula is substantiated in detail in [22]. According to the Braggeman formula, for our case we get:

$$\begin{aligned}
 V_{cl} \frac{\varepsilon_{cl} - \varepsilon_{cl}^{bw}}{\varepsilon_{cl} + 2\varepsilon_{cl}^{bw}} + V_{bw} \frac{\varepsilon_w - \varepsilon_{cl}^{bw}}{\varepsilon_w + 2\varepsilon_{cl}^{bw}} &= 0, \\
 V_{sa} \frac{\varepsilon_{sa} - \varepsilon_{sa}^w}{\varepsilon_{sa} + 2\varepsilon_{sa}^w} + V_w^{sa} \frac{\varepsilon_w - \varepsilon_{sa}^w}{\varepsilon_w + 2\varepsilon_{sa}^w} &= 0, \\
 V_{si} \frac{\varepsilon_{si} - \varepsilon_{si}^w}{\varepsilon_{si} + 2\varepsilon_{si}^w} + V_w^{si} \frac{\varepsilon_w - \varepsilon_{si}^w}{\varepsilon_w + 2\varepsilon_{si}^w} &= 0,
 \end{aligned}
 \tag{8}$$

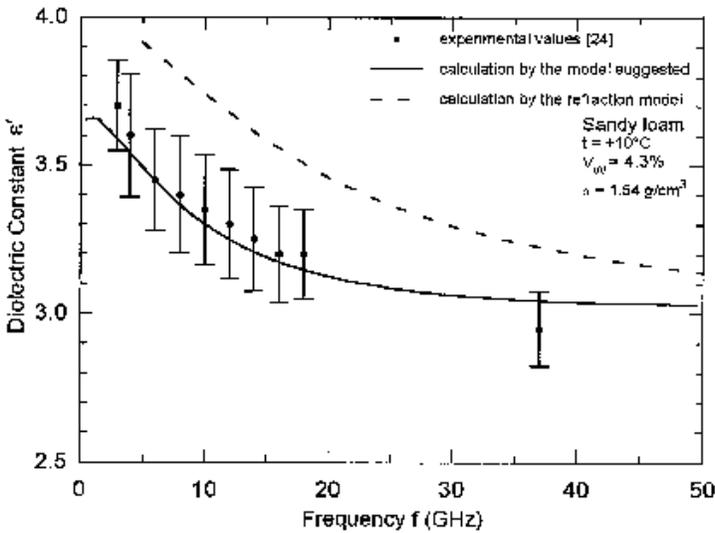
where V_{cl} , V_{sa} and V_{si} are shares of volume occupied by a clay, sand and silt particle, respectively; V_{bw} , V_w^{sa} and V_w^{si} are share of volume occupied by a bound water film covering a clay particle, by free water films covering sand and silt particles, respectively.

Thus, the model of ε_{eff} of wet soil considered in this chapter (equations (7) and (8)), takes into account the structure of soil as well as free and bound water in it. Determination of soil structural parameters necessary for the retrieval of ε_{eff} is described in detail in [22].

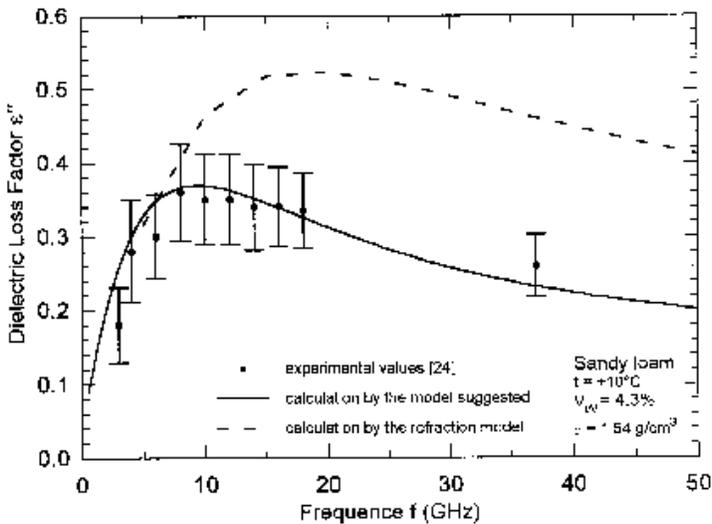
4. COMPARISON OF MODEL CALCULATIONS AND EXPERIMENTAL DATA

Model calculations of ε_{eff} of wet soils have been compared to experimental data given in [4, 23, 24]. These papers deal with laboratory experimental determination of dielectric constant of various soils at frequencies from 3 to 37 GHz in a broad range of temperature and wetness. Model calculations employed real structural parameters of soils which are also represented in [4, 23, 24]. Comparisons showed good agreement of theoretical calculations and experimental data. Some of the results are given below.

Figures 3(a), (b) and 4(a), (b) show model calculations and experimental dependencies [24] of real (a) and imaginary (b) components of dielectric constant of wet soil on radiation frequency for sandy loam at a soil temperature of +10°C, volumetric wetness of soil $V_w = 4.3\%$ (Fig. 3) and $V_v = 24.3\%$ (Fig. 4), density of dry soil of 1.54 g/cm³ and the following fraction weight composition of soil: $M_{sa} = 51.51\%$, $M_{si} = 35.06\%$, $M_{cl} = 13.43\%$. In compliance with the fraction composition of the soil as well as in line with the suggested

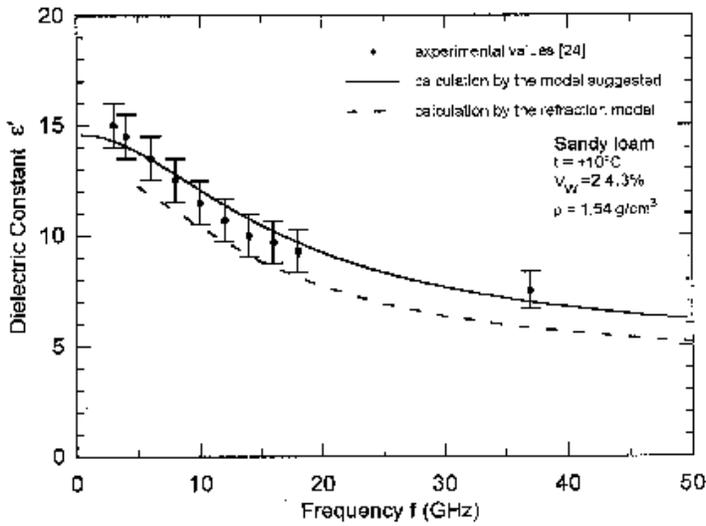


(a)

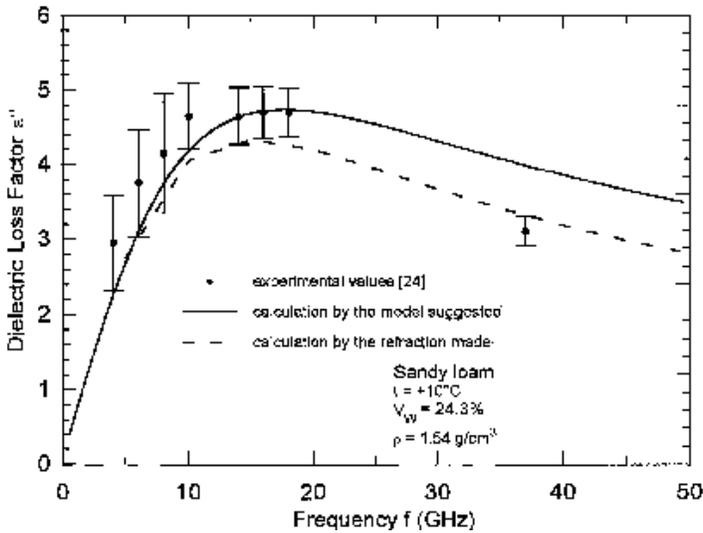


(b)

Figure 3. Frequency dependencies of real (a) and imaginary (b) components of dielectric constant of sandy loam at soil volumetric wetness of 4.3%.



(a)



(b)

Figure 4. Frequency dependencies of real (a) and imaginary (b) components of dielectric constant of sandy loam at soil volumetric wetness of 24.3%.

model, at low wetness (4.3%), all water in the soil is bound, while at high wetness (24.3%), it is free.

Experimental values in Figs. 3, 4 are given with corresponding measurement errors which for the real component of dielectric constant constituted not more than 5% for the whole range of frequencies, wetnesses and soil temperatures, while for the imaginary component they ranged 10–90% depending on soil wetness and temperature for frequencies ≤ 18 GHz, and 5–10% for frequencies of 18–37 GHz [23, 24].

For comparison, we show in Figs. 3 and 4 curves calculated according to the refraction model which is widely used to retrieve ε_{eff} of wet soils at frequencies below 10 GHz [1] but does not take into account bound water.

Analysis of dependencies presented in Figs. 3, 4 brings us to the following conclusions. At low soil wetnesses (less $\max(V_{bw})$ for the model suggested), an ε_{eff} model should take bound water into account. This is proved by the difference of dependencies calculated by the suggested and the refraction models at low soil wetness (4.3%), and their virtual identity at high soil wetness (24.3%). This confirms our suggestion stated in the first section of the present article and considered by our model, that with growing wetness, dielectric properties of bound water approach those of free water. This conclusion is illustrated in Fig. 5 which shows frequency dependencies of bound water dielectric constant in sandy loam calculated by (6) at a temperature of $+10^\circ\text{C}$ and different volumetric wetnesses of soil: 1.4, 4.3 and 24.3%. Notice, that frequency dependence of bound water dielectric constant at the wetness of 24.3% is identical to that of free water. The given curves show that with growing wetness, frequency dependence ε_{bw} approaches frequency dependence ε_w .

Experimental [23] and theoretical dependencies of real and imaginary components of ε_{eff} of sandy loam ($M_{sa} = 51.51\%$, $M_{si} = 35.06\%$, $M_{cl} = 13.43\%$, 1.54 g/cm^3) and silt loam ($M_{sa} = 30.63\%$, $M_{si} = 55.89\%$, $M_{cl} = 13.48\%$, 1.5 g/cm^3) on volumetric wetness of soil at a temperature of $+22^\circ\text{C}$ and frequencies of 4 and 18 GHz are presented in Fig. 6(a), (b). To make the picture more understandable, measurement errors are not shown here, their values are the same as in Figs. 3, 4 [23]. In the Fig. 6(a), (b) vertical dotted line is the wetness $V_w = \max(V_{bw})$; for both soil $\max(V_{bw}) \approx 26\%$. According to the suggested model of soil permittivity and soil bound water dielectric constant, this is the wetness where bound water becomes free.

It is necessary to underline, that the suggested model of ε_{eff} assumes the presence of bound water in a soil only when there is

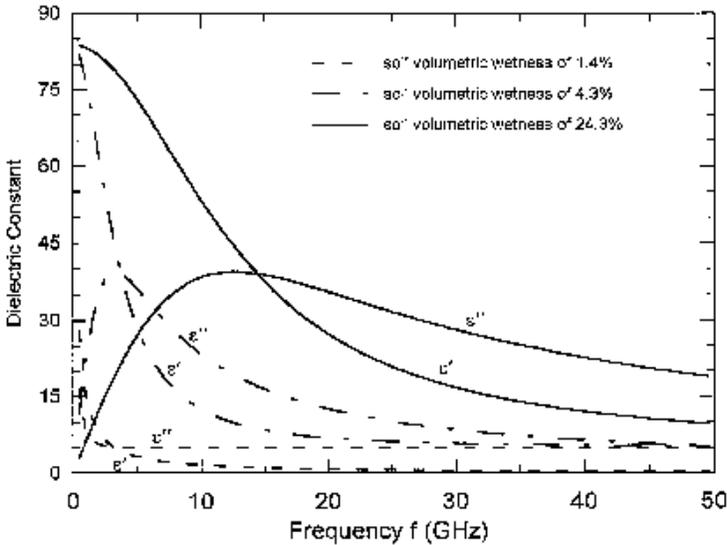
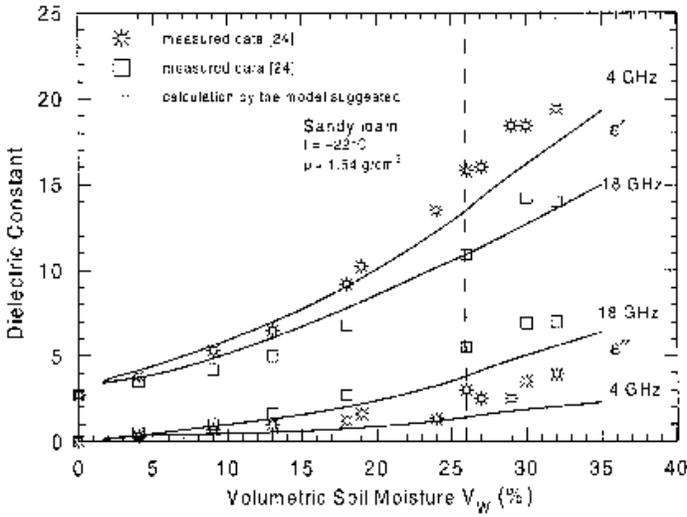


Figure 5. Frequency dependencies of bound water dielectric constant of sandy loam calculated by the model.

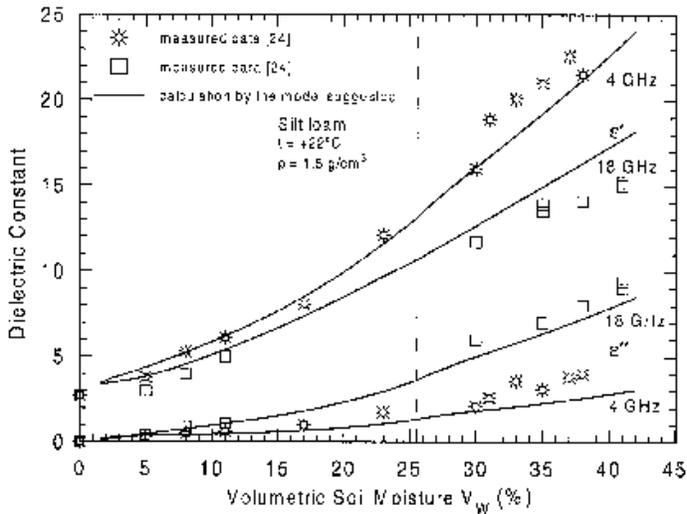
a clay fraction in that soil. In real soils, bound water films cover other particles as well (sand and silt). However, if we recall that the maximum thickness of bound water is 10 monomolecular layers (2.8×10^{-7} cm), than, according to estimates [22], the amount of bound water on sand and silt particles is less than 0.1% and we may neglect it in the model. Fig. 7 gives a confirmation of that showing experimental dielectric constants of sand [2] and theoretical dependencies ϵ_{eff} on wetness of this soil calculated by our model at a frequency of 5 GHz. Figure 8 displays experimental dependencies of sand permittivity on wetness obtained at Altai State University under the supervision of V. L. Mironov. Experiments were conducted at a frequency of 1.11 GHz for a sand of a density of 1.7 g/cm^3 and of a mean particle diameter of 0.005 cm. The same Figure shows dependencies calculated according to the suggested model. Calculations and measurements do agree well in the whole interval of wetness.

A few remarks should be made on the limits of applicability of the suggested model of bound water dielectric constant in soil, and on the agreement of values of ϵ_{bw} calculated by the model with real values.

Certainly, the model of dielectric properties of soil bound water described here has its drawbacks. There still remain the problems of bound water dielectric constants in the static case and at high



(a)



(b)

Figure 6. Experimental and theoretical dependencies of sandy loam (a) and silt loam (b) dielectric constant on volumetric wetness at frequencies of 4 and 18 GHz. Dotted line is the wetness where bound water becomes free.

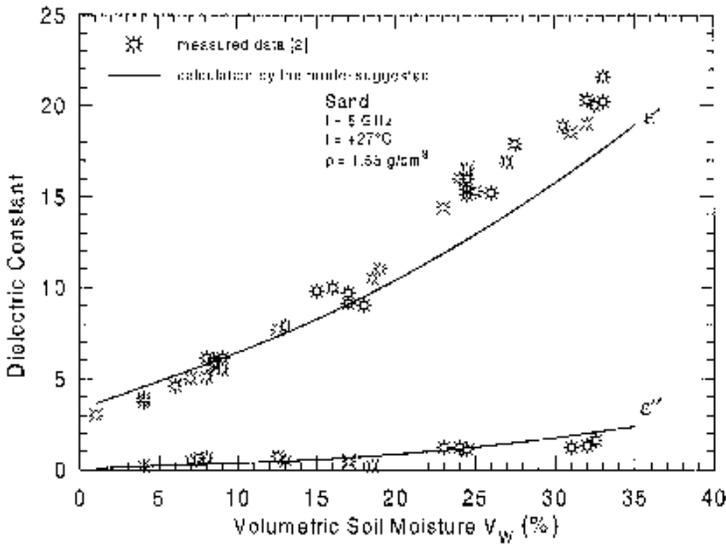


Figure 7. Sand dielectric constant dependencies on volumetric wetness at a frequency of 5 GHz.

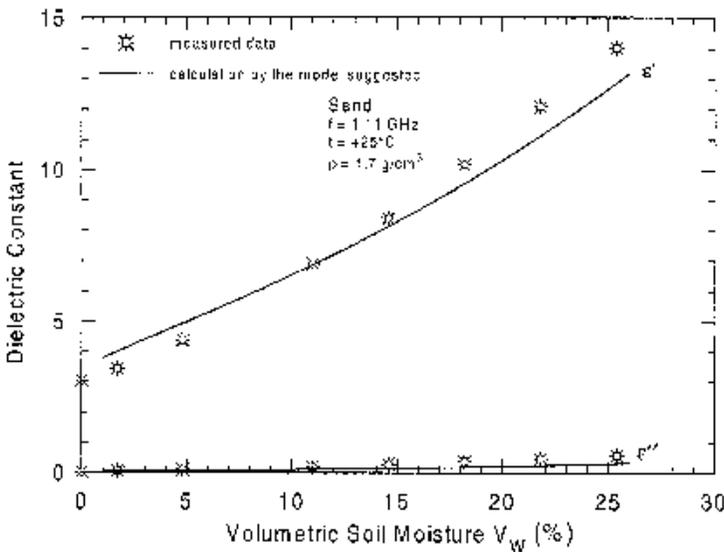


Figure 8. Sand dielectric constant dependencies on volumetric wetness at a frequency of 1.11 GHz.

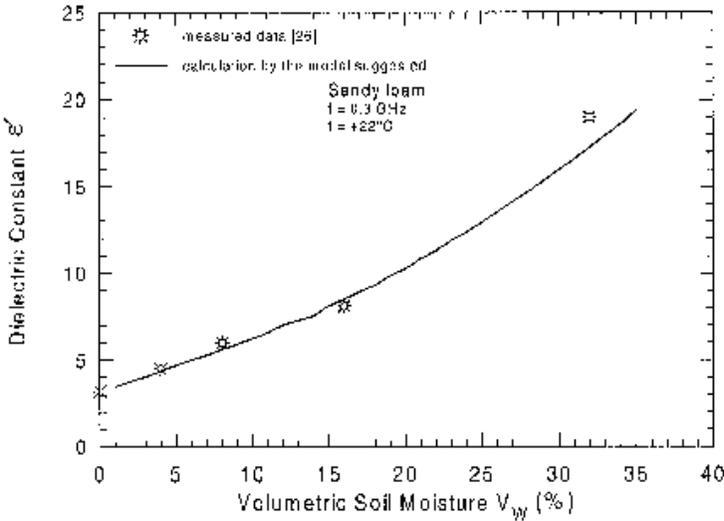


Figure 9. Sandy loam dielectric constant dependencies on volumetric wetness at a frequency of 0.3 GHz.

frequencies, dielectric constants which we assumed equal to the dielectric constant of free water in our model. Also unknown is the dependence of relaxation wavelength of bound water on temperature. Further, some grounds exist to suppose that bound water permittivity dependence on radiation frequency has another, more complex than Debye shape. Unfortunately, for the time being there is no way to investigate these problems because of the lack of experimental data.

As was noted above, the model makes it possible to describe frequency dependence of dielectric constant of various soils at low wetness (Figs. 3, 4). According to the model of ϵ_{bw} with the decrease of radiation frequency, bound water dielectric constant comes closer to that of free water (see Fig. 2). This fact is especially well illustrated in Fig. 2(a): at a frequency of 0.3 GHz bound water dielectric constant in sandy loam equals free water dielectric constant almost in the whole wetness range. And values of ϵ_{eff} for this soil calculated depending on wetness at the frequency of 0.3 GHz agree well with experimental data of [25]: Fig. 9. The growing proximity of bound and free water dielectric constants under decreasing radiation frequency explains why the refraction model (which disregards bound water) gives good description of dielectric properties of wet soils at frequencies less than 10 GHz.

According to the suggested model of ϵ_{bw} , bound water dielectric

constant depends on the thickness h of water film covering clay particles of the soil. However, this film thickness cannot be less than one water molecule diameter (2.8×10^{-8} cm [13]). This means, that the approximation $\tau_{bw}(+27^\circ\text{C})$, (1), will correspond to experimental data (see table) only at $h \geq 2.8 \times 10^{-8}$ cm. Therefore, if the volume of water in soil is less than a certain “critical” amount, meaning wetness, at which all water could be uniformly distributed in the form of films of thickness of 2.8×10^{-8} cm around particles of soil, then the definition of ε_{bw} assumed for this model will not be correct. At soil wetness below that “critical” value, water will stay in the shape of patches on soil particles and part of particle surfaces will not be covered by it [26]. Apparently, in this case we can speak about the so-called “strongly bounded” water, dielectric properties of which are close to those of ice [1, 10].

It is noteworthy that all calculations made and presented in this work were performed under the condition $h \geq 2.8 \times 10^{-8}$ cm.

5. CONCLUSION

Calculations of permittivity based on the suggested model of ε_{eff} well agree with experimental data in the considered frequency range (0.3–37 GHz) for various soils and at various wetnesses and temperatures. This agreement was reached due to the consideration given in the model of ε_{eff} to structural properties of a soil as well as due to the suggested model of soil bound water dielectric constant.

The model of dielectric properties of soil bound water discussed here made it possible to obtain an explanation for the region of transitional wetness as well as to describe dielectric properties of soils of low wetness.

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