Predicting Microwave Complex Dielectric Constant of Water-Surfactant Mixtures

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Abstract- Low dielectric constant, low conductivity surfactant X-100 was mixed with deionized water to form mixtures that had a wide range of complex permittivity. Two parallel mixing rules were used to predict the complex dielectric properties of the mixture in the microwave frequency range: a simple 2-component mixing rule and a 3-component mixing rule in which water was treated as comprised of free and bound waters. Experimental results show that the incorporation of bound water into the mixing rule improves the prediction to a great extent. A diagram to help predicting the bound water fraction for the mixture is also given in this paper.

Indexed Terms- artificial tissue emulating phantoms, dielectric constant, loss factor, microwave, surfactant.

I. INTRODUCTION

Artificial tissue emulating (ATE) phantoms are objects designed to replace human tissues in tests that may inflict unknown or uncertain consequences. Depending on tests requirements, these ATE phantoms are designed to have similar thermal, optical, electrical, electromagnetic, or acoustic properties to their target human tissues [1]. For example, a microwave imaging system can be useful for the emergent detection of brain stroke or early breast cancer detection. In developing such a system, electromagnetic interaction between microwave and human body must be fully understood. To validate the performance and safety of the system, a great amount of tests must be carried out before conducting any human subjects research. The development of ATE phantoms that are both effective and low-cost will be beneficiary for the testing purpose of such a system. In addition to a microwave imaging system, the study of interaction of electromagnetic waves with human body is also important to cellular phone development, radio base station installation, wearable antenna design for body area networks, and implantable antennas, etc. [2].

ATE materials for testing microwave apparatus can be classified into 4 types: liquid, gel, semisolid and solid [1]. Among them, the liquid type materials have the advantages of easy preparation, versatility, long shelf life and good property stability. Phantoms made of liquid type materials are most useful for mimicking tissues with high water content; and water can be used as the main ingredient. For tissues of low water content or with high amount of low-permittivity fat, like bone and breast, low-permittivity substances such as alcohol, sucrose, polyvinylpyrrolidone and octylphenol ethylene oxide condensate (a poly(ethylene glycol) derivative, trade name Triton X-100) can be used[3,4]. In situations that a certain shape is specified or more appropriate in the test, a container made of plastic film can be easily tailored. Also commercial phantom shells are available in the market for certain tests.

Triton X-100 is a low cost non-ionic surfactant. It is soluble in polar solvents such as water and alcohol. It is also soluble in nonpolar solvents such as toluene and xylene. By measuring the complex permittivity of mixtures of different proportions of deionized water (DI water) and X-100 in broadband electromagnetic characterization in the 0.5–12 GHz frequency range, it was found the mixtures were able to satisfactorily mimic different types of breast tissues [3]. To evaluate the health risks posed by mobile-telecommunication equipment, values of the dielectric property at various frequencies of a liquid phantom equivalent to whole-body tissues are specified by international organizations. X-100 and DI water are among the ingredients recommended by these international organizations for preparation of liquid phantoms to meet the requirements for tests and measurements [5].

Usually when a new device is designed to inspect or to target a certain human tissue, then there is a need for a new ATE phantom. Commonly a time-consuming, trial-and-error approach is required to develop a new phantom. A time- and cost-effective method for developing a new ATE phantom will be very valuable. X-100 is a low permittivity material, while in contrast, DI water is a high permittivity material. The mixtures of the two can be used to make phantoms to mimic a wide range of human tissues. This work aims to seek if there is a mixing rule that can be used to effectively predict the complex permittivity of the DI water/X-100 mixture.

II. EXPERIMENTALS

Triton X-100 was purchased from First Chemical Works and has a room temperature density of 1 g/cm^3. 5 compositions of DI water/X-100 mixtures with weight ratios of 85/15、80/20、75/25、70/30、65/35 were prepared using a laboratory overhead stirrer. The complex permittivity of each composition was measured in the frequency range from 5 to 10 GHz at 298.15 K using an Agilent 8720ES Vector Network Analyzer (VNA) equipped with a coaxial dielectric probe. The frequency dependent complex permittivity is expressed as $\varepsilon(\omega) = \varepsilon'(\omega) - j\varepsilon''(\omega)$, where ε' and ε'' denote the real and imaginary parts of the complex permittivity, and ω is the angular frequency. The experiment data will be presented as dielectric constant (relative permittivity) $\varepsilon_r' = \varepsilon'/\varepsilon_o$ and loss factor $\varepsilon_r'' = \varepsilon''/\varepsilon_o$, where ε_o is the permittivity of free space. When the static conductivity is negligible, the loss factor is related to the effective conductivity σ by $\sigma = \varepsilon_r''\varepsilon_o\omega$.

III. RESULTS AND DISCUSSION

The simplest approach to estimate the material properties of a mixture is to assume that there is no interaction between components, so the mixture property is the volume-weighted average of the component properties. This simple mixing rule can then be expressed as:

$$\varepsilon_r = \varepsilon_{rw}v_w + \varepsilon_{rx}v_x \tag{1}$$

, where ε_r, $\varepsilon_{rw}$and ε_{rx} are the relative complex permittivities of the mixture, water and X-100, respectively, v_w and v_x are the volume fractions of water and X-100, respectively. The second approach adopted here is to take the interaction between water and the polar group of X-100 into account. Because the polar part of X-100 interacts favorably with water molecules, those water molecules in the vicinity of the X-100 hydrophilic groups are different from those in the bulk in terms of dielectric responses. The polarity and relaxation behaviors of water molecules adhering to X-100 change drastically, which in turn will lead to a drastic change in dielectric properties. The water can then be divided into two parts: free water and bound water[6]. Bound water refers the portion of water molecules that are tightly hydrogen-bonded to the polar group of X-100. Free water refers to the portion of water molecules that are unaffected by X-100. The modified mixing rule can then be expressed as:

$$\varepsilon_r = \varepsilon_{rw}v_{wf} + \varepsilon_{rwb}v_{wb} + \varepsilon_{rx}v_x \tag{2}$$

, where $\varepsilon_{rwb}$the relative complex permittivity of is bound water, v_{wf} and v_{wb} are the volume fractions of free and bound water, respectively. The values of ε_{rw}(relative complex permittivity of water) at temperature T (in K) and frequency f are calculated using[7]:

$$\varepsilon_{rw} = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + j2\pi f\tau} \tag{3}$$

, where τ is the relaxation time and can be calculated using:

$$\tau = 3.745 \times 10^{-15}[1 + 7 \times 10^{-5} \cdot (T - 300.65)^2] \cdot exp(2295.7/T) \tag{4}$$

, ε_∞ and ε_s are limits of the dielectric constant at high and low frequencies, and are 5.085 and 78.39, respectively at 298.15 K. The values of ε_{rwb} (relative complex permittivity of bound water) are calculated using[6]:

$$\varepsilon_{rwb} = 2.9 + \frac{55}{1 + (jf/1.8\times10^8)^{0.5}} \tag{5}$$

Although (5) was obtained from fitting the data measured in the frequency range 0.1-20 GHz at 295.15 K, it is still used in this paper for the data obtained at 298.15K because the temperature difference is small. Fig. 1 shows the behaviors of the dielectric constant and the loss factor as functions of frequency of water, bound water and X-100. The data for X-100 are obtained experimentally, while those for water and

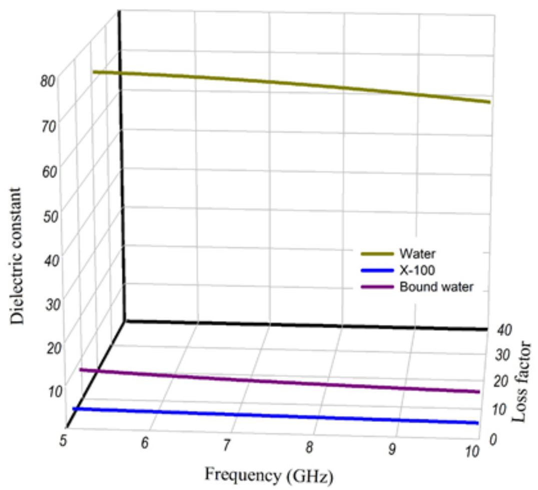

Fig. 1 Dielectric constant and loss factor as functions of frequency for water, bound water and X-100.

bound water are calculated using (3) and (5), respectively. X-100 is much less polar than water, and has much lower values of dielectric constant and loss factor. Bound water is also much less polar than free water, and has values higher than but closer to those of X-100. The dielectric constants of all the three components decrease with increasing frequency because some of the polarization mechanisms fail to follow the field alternation at higher frequencies. The loss factors of bound water and X-100 also decrease with increasing frequency because the decrease of acting polarization mechanisms leads to lower polarization loss. It is interesting to see that the loss factor values of bound water are also much closer to those of X-100. The loss factor of water increases with increasing frequency because the frequency range is within its relaxation frequency range.

The mixing rules in (1) and (2) are based on volume fractions, while the sample designation uses the weight ratio. The volume fraction values (v_x) of X-100 are 0.142, 0.189, 0.238, 0.286 and 0.335, respectively, for mixtures 85/15, 80/20, 75/25, 70/30 and 65/35. It is further assumed that the sum of the volume fractions of free water and bound water in (2) are equal to the volume fraction of water in (1), i,e., $v_w = v_{wf} + v_{wb}$. The values of v_{wf} and v_{wb} for each composition are determined by finding the minimum values of $\sum_i (\varepsilon_r - \varepsilon_{r,exp})_i^2$, where $\varepsilon_{r,exp}$ is the experimental complex permittivity and ε_r is the complex permittivity calculated using (2). Fig. 2 shows the

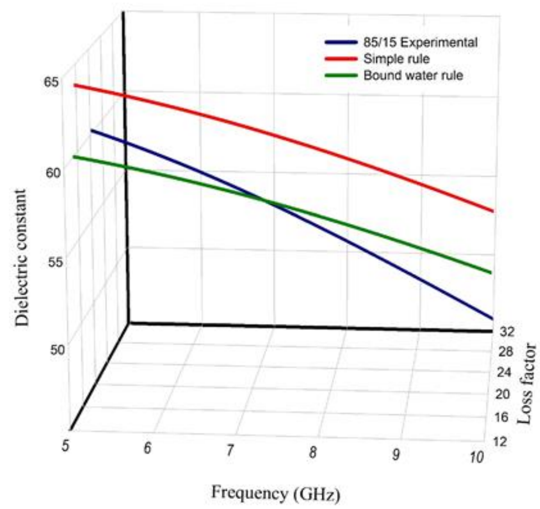

Fig. 2 Dielectric constant and loss factor as functions of frequency for mixture 85/15.

experimental complex values, those predicted by (1) and by (2) for mixture 85/15. In the figure, simple rule represents the curve calculated by the using (1), the simple mixing rule, while bound water rule represents the curve calculated using (2), the modified mixing rule. In the 3-D figure, the curve calculated using (2) lies much closer to the experimental curve. The incorporation of an additional parameter, bound water volume fraction v_{wb}, into the mixing rule greatly enhanced the accuracy of prediction. The increase in workload for finding the optimal v_{wb} is minimal

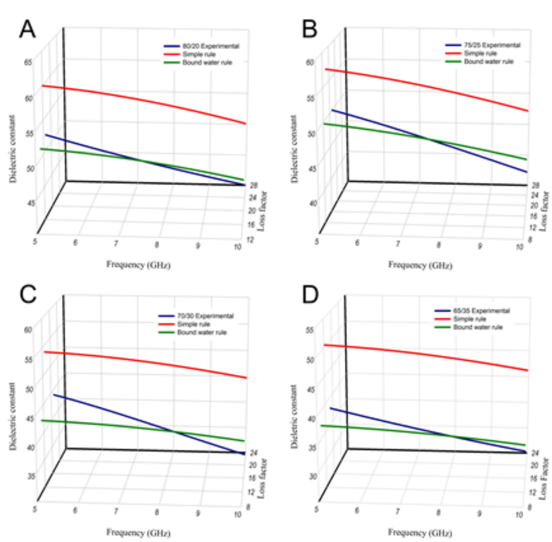

Fig. 3 Dielectric constant and loss factor as functions of frequency for mixture (A) 80/20 (B) 75/25 (C) 70/30 (D) 65/35.

considering that finding a minimum is a simple task when there is only one unknown.

Fig. 3 shows the result of predictions using the two models for the remaining compositions. A high degree of success for the predictions by using (2), the bound water mixing rule over those by using (1), the simple mixing rule is seen. Although the complex dielectric properties of bound water might not be the same for different mixture systems and could also be composition-dependent. For the water-X100 mixture system, using (2) together with (5) worked very well for X-100 in the range of 15 – 35 wt%.

To assist the prediction of dielectric properties of water/X-100 system, the obtained bound water volume fractions were plotted against water weight fractions of the mixtures and a smooth curve was drawn, as shown in Fig. 4. It is found in this figure that bound water fraction decrease with increasing water weight fraction. This is reasonable because the mixture should have a higher fraction of bound water when there exists a higher fraction of X-100. The modified mixing rule could speed up the process of developing a new ATE phantom since it can make a sound prediction of the dielectric properties of a mixture with various compositions. The methodology could work for developing phantom formulations as long as water is a major ingredient.

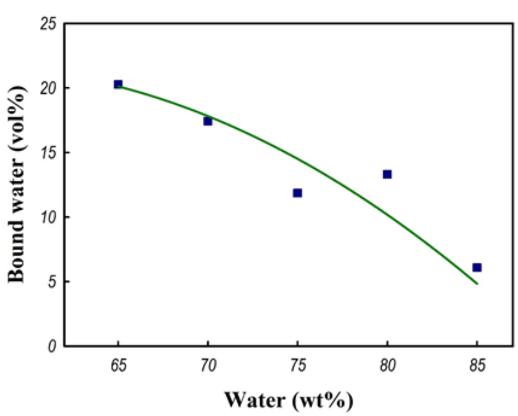

Fig. 4 The fitted bound water volume fractions for mixtures of different water weight fractions.

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