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Determination of microscopic optical properties of agar and Zerdine phantoms at 635 nm using Kubelka-Munk function approach: a numerical study

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ABSTRACT

Since the precise and accurate determination of the optical properties of materials is very important for the development and application of optical technology, the investigation of the optical properties of biological tissues with tissue-like phantoms is an important research field in the applications of lasers in medicine. In this study, after directly determining the macroscopic optical properties of the agar and Zerdine phantoms at 635 nm, including the absorbance, transmittance, reflectance, refractive index, and total attenuation coefficient with the single integrating sphere test apparatus; the microscopic optical characterization of these two different soft tissue phantoms were realized at 635 nm by using the Kubelka-Munk function approach. For this, the microscopic optical parameters, which are the absorption coefficient, scattering coefficient, reduced scattering coefficient, and penetration depth, were calculated over these determined macroscopic optical properties.

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1. INTRODUCTION

The materials, in line with their usage purposes, can be characterized in terms of optical, thermal, mechanical, acoustical, and electrical properties. Phantoms are also used as reference objects in preclinical tests for medical purposes. The ability of phantoms to be used repeatedly by mimicking the properties of living tissues provides great advantages, particularly in medical research. The use of tissue-like materials is also common in biophotonic research. While parameters such as speed of sound, characteristic acoustic impedance, acoustic attenuation coefficient, and acoustic backscatter coefficient are examined in acoustical characterization, optical parameters such as absorption coefficient, scattering coefficient, and anisotropy factor are measured in optical characterizations for phantoms [1]–[3].

The Kubelka-Munk model is a theoretical reflectance model that is commonly used in optics. In this model, it is assumed that some light passing through a homogeneous sample is scattered and absorbed in two directions; thus, the light is weakened. The Kubelka-Munk model is a two-flux approach to general radiation transfer theory. The propagation of the up and down fluxes is characterized by the Kubelka-Munk scattering and absorption coefficients, which are designated as S and K, respectively. The definition of the optical properties of light-scattering materials has enabled the extensive use of radiation transfer models. One of the most successful and simplest models is the Kubelka–Munk model. Using this model, the optical properties of particulate films under diffused illumination can be estimated from the effective absorption and scattering coefficients of the material. To examine materials, the Kubelka–Munk model has many applications, such as in papers, paints, pigmented plastics or polymers, decorative and protective coatings, solar-absorbing pigments and paints, human tissue, leaves, biological systems, crystalline materials, melting of solids, powders, fibrils and wool, thermal insulation, optical properties, medical physics, and atmospheric physics. In this model, it is assumed that the optical properties of the coating are described by two constants: absorption and scattering coefficients [4]–[14].

Optical characterization of the materials is carried out by determining their microscopic optical properties. In this study, the microscopic optical properties, which are the absorption coefficient, scattering coefficient, reduced scattering coefficient, and penetration depth, were determined at 635 nm for the first time using the Kubelka-Munk function approach over the macroscopic optical properties measured using a single integrating sphere system. The microscopic optical properties of the agar and Zerdine phantoms were calculated using basic macroscopic optical properties data from our previous study [15]. Therefore, it would be more advantageous to work with mathematical models that use current similar situations, rather than more complex methods. In this respect, the present work includes an important innovation in phantom studies.

2. RESEARCH METHOD

2.1. Tissue-mimicking materials/phantoms and their preparation

Tissue-mimicking materials (TMMs) are generally used in medical research because of their ability to simulate biological soft tissues. In our study, two types of tissue-mimicking materials, Zerdine, and agar were used. While the Zerdine phantom is used as a reference test material in the quality control of ultrasonic imaging systems, the agar phantom is generally used in the ultrasonic research field. The Zerdine phantom was produced using the formulation in Zerhouni and Rachedine's patent [16]. The agar phantom was prepared by creating a 250 ml solution of 0.4 M ZnCl2 and 2% agar by the weight of the initial water [17].

2.2. Optical measurements tools

Optronics branded VA-I-400-635 model 635 nm wavelength red colored solid-state diode laser, Ophir branded StarBright model optical power meter, Ophir branded 3 A type thermal sensor, and Thorlabs IS200 model 2" integrating sphere was used for the optical measurements such as absorbance and transmittance.

2.3. Calculation of macroscopic and microscopic optical properties

The related macroscopic formulas used in the calculations for the absorbance, transmittance, reflectance, refractive index, and optical linear attenuation coefficient are as (1)-(6).

R+T+A =1 or %R+%T+%A = %100 [18] (1)

Absorbance, A; A=-log(I/I_0)=-log(T)=2-log(%T) [19] (2)

Transmittance, T; T = I/I_0 [19] (3)

Reflectance, R; R=1-(A+T) [18] (4)

Reflectance, $R = \frac{(n-1)^2}{(n+1)^2}$, [18] (5)

Where n is the refractive index.

$I = I_0 e^{-\mu x}$, $\mu = -\frac{\ln \frac{I}{I_0}}{x}$ [20] (6)

Where μ is the linear or total attenuation coefficient.

The related microscopic formulas used in the calculations of the absorption coefficient, scattering coefficient, reduced scattering coefficient, total attenuation coefficient, and effective penetration depth are as follows:

a. The Kubelka-Munk function is given by (7).

$F(R) = \frac{(1-R)^2}{2R} = \frac{k}{s}$ [21] (7)

Where R = Reflectance, k = Absorption Coefficient, s = Scattering Coefficient.

b. The total attenuation coefficient is described by (8).

$$\mu = \mu_t = \mu_a + \mu_s \text{ [22]} \quad (8)$$

Where μ_a is Absorption Coefficient and μ_s is Scattering Coefficient. That is, k=μ_a and s=μ_s can be matched using (7) and (8).

c. The reduced scattering coefficient (μ_s') is defined by (9).

$$\mu_s' = (1-g)\mu_s \text{ [23]} \quad (9)$$

Where "g" is the anisotropy factor. The "g" value of the phantoms was fixed at 0.9, which is the anisotropy factor of the human tissue in the UV and near-infrared spectra.

d. The effective penetration depth; Deff, is described by (10).

$$D_{eff} = \frac{1}{\sqrt{3\mu_a[\mu_a+\mu_s(1-g)}} \text{ [24]} \quad (10)$$

3. RESULTS AND DISCUSSION

3.1. Optical properties measurements

The macroscopic optical properties of the following soft tissue phantoms, such as absorbance, transmittance, reflectance, refractive index, and total attenuation coefficient, were calculated at 635 nm in our previous paper with a single integrating sphere test setup, as shown in Table 1 [15]. By using these macroscopic optical properties, microscopic optical properties, including the absorption coefficient, scattering coefficient, reduced scattering coefficient, total attenuation coefficient, and effective penetration depth, were calculated at 635 nm via the Kubelka-Munk function approach. We calculated μ_t from interpolation, and we know R is the reflectance value; then, we can solve these two equations (7) and (8) and find μ_a and μ_s. Therefore, the microscopic optical properties of the Zerdine and agar phantoms, such as the absorption coefficient, scattering coefficient, reduced scattering coefficient, total attenuation coefficient, and effective penetration depth, were calculated as shown in Table 2.

Table 1. The measured optical properties of the Zerdine and agar phantom as average with the single integrating sphere measurement method

Phantom	Transmittance T	Absorbance A	Reflectance R	Refractive Index	Total Attenuation Coefficient (cm^{-1})
Zerdine	0.91±0.03	0.04±0.01	0.05±0.01	1.58±0.08	0.03±0.01
Agar	0.44±0.21	0.41±0.27	0.15±0.09	2.26±0.64	0.91±0.10

Table 2. The calculated microscopic optical properties of the Zerdine and agar phantoms as average at 635 nm

Phantom	Absorption Coefficient, μ_a, cm^{-1}	Scattering Coefficient, μ_s, cm^{-1}	Reduced Scattering Coefficient, μ_s', cm^{-1}	Total Attenuation Coefficient, μ_t, cm^{-1}	Effective Penetration Depth, D_{eff}, cm
Zerdine	0.025±0.011	0.003±0.001	0.001±0.0004	0.028±0.012	22.655±12.253
Agar	0.642±0.074	0.266±0.031	0.053±0.006	0.908±0.104	0.865±0.101

4. CONCLUSION

In this study, the microscopic optical properties of agar and Zerdine phantoms, such as the absorption coefficient, scattering coefficient, reduced scattering coefficient, total attenuation coefficient, and effective penetration depth, were calculated at 635 nm over the macroscopic optical properties using the Kubelka-Munk function approach. In the present work, macroscopic and microscopic optical properties of phantoms are important distinguishing properties in the optical characterization of materials over two distinct phantom examples. Therefore, these optical properties can provide very precious information to medical optical device developers for the development and applications of optical technology. By using the Kubelka-Munk function approach, similar studies can be carried out on different phantoms in future studies.

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