Numerical modelling of radiant energy extinction by water medium containing bubbles and particles of various natures

O V Shefer¹, V V Loskutov¹

¹ Tomsk Polytechnic University, 30, Lenina ave., Tomsk, 634050, Russia

E-mail: deonold@gmail.com

Abstract. In the framework of the Mie theory, we developed a numerical model of weakly absorbing medium, containing particles having an arbitrary chemical composition. This model can be applied to the study of the extinction characteristics of the optical radiation by a water layer with gas bubbles or volume-shape particles. The results of the numerical experiment illustrate changes in optical properties of the water due to the presence of bubbles or solid particles. The work displays some calculations of the extinction efficiency factor, the extinction coefficient, and transmission function at visible wavelengths. The influences of concentration and sizes of gas bubbles on the extinction characteristics of optical radiation are illustrated. Features of the extinction of radiant energy are discussed as dependent on a size parameter and a complex index of refraction of scatterers.

1. Introduction

All over the world, a large amount of attention is given to an investigation and mastering of marine areas [1–3]. This is due to the solution of problems of rational nature management and the need to control the environment. The systems of laser sensing of aquatic environments are actively employed to research the water medium. Sensing data are used for diagnosis of a composition of a light-scattering layer. The change of radiation parameters is associated with features of scattering and absorption by the inhomogeneities of water environment. Nowadays, acoustic sensing is most widely used for study of the ocean [3]. The mechanisms of interaction, leading to scattering of electromagnetic radiation, differ significantly from features of the sound scattering. An optical system allows the monitoring of a composition of aquatic environment with relatively small components (particle sizes are different from the wavelength of not more than several orders of magnitude); it is not possible to detect such components by using acoustic systems. By using electromagnetic radiation, hydro-lidar systems can significantly extend the capabilities of remote sensing techniques of the ocean.

In this work, we propose a numerical model applicable to the optical methods of investigation of the water layer containing some inhomogeneities. Both bubbles and volume-shape particles, having arbitrary optical properties (i.e., any complex index of refraction), can act as inhomogeneities. By laser sensing of seawater, a visible light can penetrate to depths of hundreds of meters. This should be taken into account in a numerical experiment. It is possible to note windows of transparency of water in the infrared range, where the absorption index is not high, but nevertheless, is not a negligible value [4, 5].

By using this model, we performed some numerical study of the characteristics of the extinction of the optical radiation. In this paper, we focus on the discussion of the calculation results for the

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extinction efficiency factor, the extinction coefficient and the transmission function of the optical radiation for the water medium containing gas bubbles.

2. Methods of calculations

Let us consider a water layer with thickness *h*. The refractive index of water is denoted as *m*. Water layer contains particles of volume shapes. The spherical particle is selected as the model of the scatterer. This model is quite suitable for the numerical representation of both small and large randomly oriented particles [6]. Let *a* be the radius of the spherical particle and λ be the wavelength of the incident radiation. By $\tilde{n} = n + i \chi$, let us denote a complex index of refraction of the particle, where *n* is the refractive index and χ is the absorption index.

Let us define the characteristics of the extinction of the electromagnetic radiation for volume-shape particles in the framework of the Mie theory [6]. For this purpose we use the solution of the scattering problem of the plane wave on the sphere. This solution allows us to determine the optical single-scattering characteristics of the volumetric particles with different sizes. The extinction for such particles is a scalar value. To calculate the extinction characteristics for the case of large preferentially oriented crystals, the vector nature of the radiation should be taken into account. The polarization properties of the extinction are most pronounced for plate and columnar crystals. There features were illustrated in our papers [7, 8].

In the case of scalar (or unpolarized) fields, the extinction cross section is given by

$$\mathbf{S}_{\text{ext}} = \frac{4 \cdot \pi}{k^2} \operatorname{Re}(\mathbf{S}(0)) \tag{1}$$

where k is the wave number. Value S is determined by the amplitude of the scattered field in the exact forward direction.

To analyze the extinction characteristics, we also used the dimensionless value such as extinction efficiency factor

$$Q_{\text{ext}} = S_{\text{ext}} / S_{\text{sq}}, \tag{2}$$

where S_{sq} is the area of the particle geometrical projection on the detector surface crystal shadow.

Modelling the extinction process of radiant energy for media requires considering the extinction coefficient. The extinction coefficient for a system of particles can be defined as

$$\alpha_{\text{ext}} = \mathbf{C} \cdot \langle \mathbf{S}_{\text{ext}} \rangle \,. \tag{3}$$

Here $\langle S_{ext} \rangle$ is the average extinction cross-section; C is the volume concentration of particles.

When the radiation beam transmits through a water layer with particles, radiation intensity decreases. To calculate the transmission function, one may use the following expression:

$$T = \exp(-\alpha_{ext} \cdot h) . \tag{4}$$

For studying the spectral-wave dependence of the extinction, it is necessary to use a priori the information on the particle nature and select acceptable wavelength ranges for laser sensing of a water medium. The proposed optical model considers a non-absorbent medium. In this medium, there are particles that can absorb and scatter light to a varying extent.

3. Results of calculations

At present, a particular interest of researchers is the problem of detection of gas hydrates and high concentrations of methane bubbles in water, which can serve as an indicator of oil and gas deposits and the fault zones, and also allow assessing the seismic activity in the earthquake prediction [2]. By

using the presented numerical model, this paper focuses on discussing the results of the calculation of radiant energy extinction by the water layer containing bubbles. In the case of single-frequency laser sensing of the aquatic environment as the most optimal, green laser stands out (wavelength of 532 nm) [9].

To calculate the optical characteristics of the medium, the input parameters were the wavelength of the incident radiation, the refractive index and the thickness of the considered water layer containing particles, and also values of the complex refractive index, the radius and the concentration of the particles.

At high concentration of methane (or other gas) in bubble, its refractive index, which is typical for the visible range of wavelengths, is practically the same as the refractive index of air. The values of the absorption index of methane bubbles were calculated with the use the spectral line parameters from databases HITRAN 2012 [10]. For a visible wavelength range, these values are negligibly small ($\chi \approx 0$), even in case of high partial pressures (hundreds of atmospheres).

Optical properties of pure water in liquid and solid state and optical properties of sea water with different salt content are slightly different [4, 5], but this difference does not affect the results of calculations of the extinction characteristics. For the visible range, $m\approx 1.31$. The values of the refractive index of water containing various kinds of impurities can differ from 1.31.

Figure 1 illustrates the results of calculation of extinction efficiency factor Q_{ext} versus value g, which is determined as the ratio of particle size to wavelength (i.e., $g=a/\lambda$) with various values of the refractive index. The figure shows that the smaller the difference between m and 1, the larger the amplitude and the period of the oscillations of $Q_{ext}(g)$. The most noticeable changes in the extinction efficiency factor are observed for particle sizes comparable to the wavelength. The larger value g, the faster the value of the extinction efficiency factor tending to its asymptotic value 2.



Figure 1. Extinction efficiency factor Q_{ext} versus ratio $g=a/\lambda$ with n=1.0001, $\chi=10^{-7}$, C =10⁸ l^{-1} , $\lambda=0.532$ µm. 1-m=1.2; 2-m=1.3; 3-m=1.4.

Figure 2 shows the results of calculating the extinction coefficient versus average particle radius *a*. The most rapid change $\alpha_{ext}(a)$ is observed for particle sizes smaller than about 10 µm at a wavelength in the visible range. Clearly, the increase in the concentration leads to a linear increase of the extinction coefficient (see Eq. (3)).

Figure 3 illustrates the results of calculation of transmission function T versus size parameter $x (x=2\pi \cdot m \cdot a/\lambda)$ with various concentrations of bubbles in the water layer. The figure shows that even at high values of the size parameter (for example, at $x\approx100$) with the concentration of bubbles less than $10^5 l^{-1}$, a 10-meter water layer can be considered as transparent. By analyzing the changes of the transmission function versus the size parameter, it is possible to estimate the concentration and the size of the bubbles, which characterize the intensity of their formation.



Figure 2. Extinction coefficient α_{ext} versus average radius of particles *a* with *n*=1.0001, $\chi = 10^{-7}$, $\lambda = 0.532 \,\mu\text{m}$, *m*=1.31. 1 – C = $10^{-6} l^{-1}$; 2 – C = $5.0 \cdot 10^{-5} l^{-1}$; 3 – C= $10^{-5} l^{-1}$.

Figure 3. Transmission function T versus size parameter $x (x=2\pi \cdot m \cdot a/\lambda)$ with n=1.0001, $\chi=10^{-7}$, $\lambda=0.532$ µm, m=1.31, h=10 m. $1 - C = 10^{6} l^{-1}$; $2 - C = 5.0 \cdot 10^{5} l^{-1}$; $3 - C = 10^{5} l^{-1}$.

As we mentioned above, the visible light can penetrate hundreds of meters into a water layer. In this regard, let us consider this range of wavelengths. Figure 4 illustrates the dependence of the transmission function versus the wavelength in the visible range with different sizes of the bubbles and their concentration per unit volume. The figure shows that the manifestation of certain features in the spectral behavior of the transmission function depends on the ratio between the sizes of the particles and the wavelength of incident radiation. In other words, according to the peculiarities of the spectral behavior of the transmission function, it can be determined the average size of the bubbles and their concentration.



Figure 4. Transmission function T versus wavelength λ with n=1.0001, $\chi=10^{-7}$, $\lambda=0.532$ µm, m=1.31, h=10 m. 1-a=0.2 µm, C =10¹⁰ l^{-1} ; 2-a=0.5 µm, C =10⁹ l^{-1} ; 3-a=0.8 µm, C =5.0·10⁸ l^{-1} ; 4-a=5 µm, C =10⁷ l^{-1} .

Let us discuss the influence of the chemical composition of the particles on the features of the extinction of light. For this, we considered the water medium containing particles with different optical properties. Figure 5 and figure 6 illustrate the extinction efficiency factor versus the size parameter with different values of the refractive index of the particles.



Figure 5. Extinction efficiency factor Q_{ext} versus size parameter *x* with *m*=1.31, χ =10⁻⁷, C =10⁸ l^{-1} , λ =0.532 µm. 1 – *n*=1.1; 2 – *n*=1.2; 3 – *n*=1.4; 4 – *n*=1.6.

Figure 6. Extinction efficiency factor Q_{ext} versus size parameter x with m=1.31, C =10⁸ l^{-1} , n=1.5, $\lambda=0.532 \ \mu\text{m}$. 1 – $\chi=0$; 2 – $\chi=10^{-2}$; 3 – $\chi=10^{-1}$; 4 – $\chi=1$.

For particles with the refractive index smaller and greater than the refractive index of the medium, the difference in the patterns of change $Q_{ext}(x)$ is shown in figure 5. When n < m, the increase in n leads to the increase in the amplitude and in the period of oscillations $Q_{ext}(x)$; and when n > m, the increase of n provides its increase in the amplitude of $Q_{ext}(x)$, but the decrease in the period of $Q_{ext}(x)$. It is obvious that the increase in the values of the absorption index of particles χ leads to smoothing of the extinction features that are caused by the microphysical and optical properties of the particles. From figure 6 it is seen that when $\chi > 10^{-1}$ and x > 20, the extinction efficiency factor is equal substantially to 2 (its asymptotic value) even at co-measurement of a particle size and a wavelength.

4. Conclusions

For numerical study of the extinction characteristics of the radiant energy passing through a water medium containing particles of different nature, the optical model is presented in the framework of the Mie theory. It is shown that the peculiarities of the spectral dependence of the extinction characteristics of radiation passing through the weakly absorbing layer of water with bubbles of gas can be used to derive the size and the concentration of scatterers. However, a nature of gas cannot be identified by evaluating light extinction characteristics. Even ultra-high gas concentration (hundreds of atmospheres) in bubbles does not affect the transmittance of visible radiation. Detections of an intense and prolonged flux of bubbles in the water may be indicative of activation of physical and chemical processes in the near-bottom areas and the possible location of gas and oil fields.

Features of the spectral behavior of the extinction characteristics are determined by the relationship between the refractive index and the wavelength of incident radiation. For the particles comparable to the wavelength of incident radiation, these features are most pronounced at lower values of the absorption index of the scatterers. By analyzing the spectral dependence of the extinction coefficient and the transmission function, it is possible to evaluate the microphysical and optical properties of the particles contained in water.

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