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Methods investigation to determine optical constants of liquid based on transmittance and reflectance spectrum

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ABSTRACT

The particle swarm optimization (PSO) was introduced to calculate optical constants of liquid based on transmittance and reflectance spectrum. Two methods, namely as particle swarm double-thickness transmittance method (PTT) and particle swarm transmittance and reflectance method (PTR), were developed by combining the PSO with the spectrometry. The comparative study of two methods was carried out with distilled water as the research object, and the experimental deviation of the two methods was evaluated. The results show that the two methods are reliable for solving optical constants of liquid with high resolution accuracy, even existing experimental deviation. Meanwhile, a deviation correction method proposed in present work reduces the effect of uneven experimental deviation on the accuracy of the two methods.

1. Introduction

The optical constants are an important parameter reflecting the optical properties of liquid, which are usually related to the density and concentration of the liquid. Other parameters, such as photothermal coefficient, are also closely related to the optical constants. Liquid optical constants play an important role in the field of material identification, analysis of pollutant content and determination of mixture concentration [1–4]. In the food industry, medical, petroleum and other industrial sectors, as well as in college experiments, the liquid optical constants are often needed to measure the concentration of liquid [5–7]. Liquid optical constants are also the key for the design of biosensor and waveguide optical modulator [8,9]. Therefore, the accurate measurement of liquid optical constants plays an important role in many scientific research fields.

On account of the application of optical constants of liquid in the above industry and engineering, considerable effort has been concentrated on directly or indirectly obtaining optical constants of liquid. There are lots of methods for the measurement of optical constants of liquid, such as optical measurement methods. Optical measurements such as photoacoustic method [10], ellipsometry [11] and photometric method [12,13] are widely used to measure the optical constants of liquid. The photometric method calculates the optical constants of liquid by reflectance (R) and transmittance (T). Single-thickness photometric method can not form closed-form equations, which should be in combination with Kramers-Kronig (K-K) relation. In the late 1970 s, Jones [14] proposed a method of combining transmittance with K-K relation to retrieve the optical constants of liquid. The calculation of K-K relation needs to know the refractive index under the known high wave number, which makes this method limit in solving the optical constants of the unknown substance. On the basis of Fresnel's law, Tuntomo et al. [15] proposed a new method (i.e. double thickness method) to predict the optical constants of liquid, which not need K-K relation. The double thickness method constructed closed-form equations by measuring the transmittance at two different thicknesses or both the reflectance and transmittance at the same thickness, which

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predicts the optical constants by solving the closed-form equations. Sani [16] determined the absorption index of liquid by simplified double-thickness method, and determined the refractive index by the K-K relation. Otanicar et al. [17] used a double-thickness transmission method to calculate the optical constants of liquid fuels, and pointed out that the transmittance measurement error has certain influence on the solution of optical constants. Khashan et al. [18] combined the transmittance with the reflectance to solve the optical constants of the medium. Li et al. [19] proposed two optical constants inversion methods based on double-thickness photometric method (i.e. SEI method and MC method). The SEI method neglects the influence of the higher order reflection term. On the basis of maintaining the integrity of the transmittance calculation formulation, the MC method uses Monte Carlo method to solve optical constants. But the convergence rate is slow when the inversion values deviate from the true values. In this case, it is necessary to use the interval approximation strategy. The existing inversion methods use the iterative idea directly and the intelligent optimization algorithm is not introduced, which leads to the slow inversion and trend of falling into local optimal solution.

In sum, optical measurement methods combined with iterative algorithm are available to obtain the optical constants of liquid. But the limitation of K-K relation and the traditional iterative methods limits the reliability of the solution of optical constants. In order to overcome this limitation, the application of intelligent algorithm is considered in the solution of liquid optical constant. The particle swarm optimization (PSO) is a new intelligent optimization algorithm based on group intelligence theory and developed by Kennedy and Eberhart [20,21]. Particle swarm optimization (PSO) is robustness, efficient and intuitive, and can be implemented in any computer language [22,23], and does not need to establish complex mathematical models, which has been widely applied in many fields [24,25].

In the present study, considering the advantages of the intelligent algorithm, two kinds of inversion models, i.e. particle swarm double-thickness transmittance method (PTT method) and particle swarm transmittance reflectance method (PTR method), are developed to obtain the optical constants of liquid. The main arrangement of the paper is organized as follows. First, taking distilled water as the research object and measure its transmittance and reflectance spectra in the wavelength 0.3-0.7 u m by TU-1901/1900 two-beam ultraviolet-visible spectrophotometer in Section 2. Then, the optical constants of distilled water by using the above two methods are calculated, and the calculated values with the data in the reference are investigated in order to judge the feasibility and accuracy of the two methods. These contents are also listed in Section 2. Finally, the effect of experimental deviation on the accuracy of the two methods is analyzed, and a deviation correction method is proposed to improve the accuracy of the two methods in practical measurement in Section 3.

2. Experimental methods

2.1. Particle swarm double-thickness transmittance method

The transmission light is transferring as the condition of the Fresnel's law and Snell's law. The transmittance of the liquid under the thickness of L_1 and L_2 can be given by

$$T_1 = \frac{[1 - \frac{(n-1)^2+k^2}{(n+1)^2+k^2}]^2 e^{\frac{-4\pi k L_1}{\lambda}}}{1 - [\frac{(n-1)^2+k^2}{(n+1)^2+k^2}]^2 e^{\frac{-8\pi k L_1}{\lambda}}} \tag{1}$$

$$T_2 = \frac{[1 - \frac{(n-1)^2+k^2}{(n+1)^2+k^2}]^2 e^{\frac{-4\pi k L_2}{\lambda}}}{1 - [\frac{(n-1)^2+k^2}{(n+1)^2+k^2}]^2 e^{\frac{-8\pi k L_2}{\lambda}}} \tag{2}$$

where n is the refractive index. k is the absorption index. λ is wavelength.

Combine Eqs. (1) and (2) to form the particle swarm double-thickness transmittance model. T_{m1} and T_{m2} are the experimental measurement values of transmittance at different thickness (L_1 and L_2). Import each particle into the Eqs. (1) and (2), and the obtained values (i.e. T_{c1} and T_{c2}) are regarded as the theoretical calculation values. Based on the above values, we can construct closed-form nonlinear equations.

$$T_{c1} - T_{m1} = 0 \tag{3}$$

$$T_{c2} - T_{m2} = 0 \tag{4}$$

Then construct the following evaluation function:

$$\sqrt{(T_{m1} - T_{c1})^2 + (T_{m2} - T_{c2})^2} \leq \varepsilon \tag{5}$$

2.2. Particle swarm transmittance and reflectance method

The reflectance of the liquid under the thickness of L_1 is given by:

$$R_1 = \frac{(n-1)^2+k^2}{(n+1)^2+k^2} + \frac{(n-1)^2+k^2}{(n+1)^2+k^2} T_1 e^{\frac{-4\pi k L_1}{\lambda}} \tag{6}$$

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