A NEW RANDOM-WALK MODEL FOR ASSESSMENT OF LIGHT ENERGY ABSORPTION BY A PHOTOSYNTHETIC MICROORGANISM

TOSHIYUKI YOKOTA, KAZUYA YASHIMA, TADAHKO TAKIGAWA AND KOJI TAKAHASHI
Department of Chemical Engineering, Yamagata University, Yonezawa 992

Key Words: Photosynthetic Microorganism, Algae, Microalgae, Light Absorption, Light Scattering, Monte Carlo Method

A new random-walk model was developed to assess light energy absorbed by a photosynthetic microorganism. The model had two parameters, which were determined from transmittance through an algae suspension obtained by opalescent plate spectrophotometry. The validity of the proposed model was confirmed by comparing experimental data of light absorption in a Chlorella ellipsoidea suspension with the computation results of a Monte Carlo simulation, and by comparing light intensities passed through the suspension by a Reinecke’s salt actinometer with those predicted by the random-walk model.

Introduction

Assessment of light energy absorbed in a photosynthetic microorganism suspension provides important information for design of a cultivator and a growth kinetics analysis of the microbe. Lambert-Beer’s law is commonly used to assess light energy absorption in a micro-algae suspension\(^2\)\(^-\)\(^4\),\(^7\),\(^8\). The law disregards the effect of light scattering by algae cells. Hence it is usable only for a dilute suspension.

To evaluate the effect of light scattering in a cultivator of photosynthetic microorganisms, Koizumi et al.\(^5\),\(^6\) solved the integro-differential equation (Boltzmann’s equation), which gives the local light intensity, by the Monte Carlo method. They assumed isotropic light scattering by a microbe cell, and used the sectional areas for absorption and for scattering which were estimated from semi-integral attenuation of a microbe suspension.

In this study, we propose a new random-walk model which considers light scattering as well as light absorption by microbe cells. The model is developed from a probability model\(^1\)\(^1\),\(^1\)\(^3\) which has been proved to be useful for assessment of light absorption in a heterogeneous solid-liquid photoreaction system. Using the Monte Carlo simulation based on the model,
we estimate light energy absorbed in a microalgal suspension and compare it with results of experimental measurement in a \textit{Chlorella ellipsoidea} suspension.

1. Random-walk Model

The model assumes that a scattering light ray travels along one of the six Cartesian coordinate directions as shown in Fig. 1(a). Here $P_f$ shows the probability for forward travel of a light ray which hits a microbe cell. Other probabilities are assumed to be same for simplification. Then it becomes $1/5$ of $(1-P_f)$. The light intensity after a collision with a cell is assumed to become $\tau$ times the prior intensity (see Fig. 1(b)). The value of $\tau$ for each wavelength represents a spectral characteristic of light absorption by the photosynthetic microorganism.

Based on this model we simulated the light scattering in a microbe suspension in the following way. First, we assume that a cubic unit block, which has a side length $l$, contains a certain number of cubic subunits with a side length $l_m$, and each subunit holds one microbe cell within it. Then a volume fraction of microbe in the suspension becomes

$$\psi = (\pi/6)d^3/l_m^3$$

If the quotient of the suspension volume $V$ divided by the unit block volume is equal to the number of subunits in one unit block, the following equation holds.

$$V/l^3 = l^3/l_m^3 = 6l^3\psi/(\pi d^3)$$

Hence, $l_m$ and $l$ can be determined from the above equations when $V$, $\Psi$ and $d$ are given.

Second, we compute the trajectory of a light ray which irradiates a unit block according to the following Monte Carlo simulation method.

1. Determine whether the light ray hits a microbe cell or not in traveling a distance $l_m$, comparing the probability of a hit by Eq. (3) with a random number.

$$P_h = (\pi/4)d^2/l_m^2$$

2. If the ray hits a cell, the direction of next travel is determined by comparison of a random number with the probability $P_f$. If the ray does not hit, it travels forward.

3. Repeat the above steps until the ray reaches a boundary of the unit block.

4. After a considerable number of iterations, sum up the light intensities of light rays which leave a surface of the unit block, and count the number of light rays. Then we obtain the scattering light intensities and the escaping probabilities assigned to each surface of the unit block as shown in Fig. 2. The light absorption in the unit block is calculated as the difference between incident light intensity and leaving light intensity.

Third, we divide the whole volume of a microbe suspension into unit blocks. A traveling light path through the suspension is now computed according to the escaping probabilities assigned to the unit block, and the light energy absorbed by microbe cells is also assessed.

2. Experimental and Results

2.1 Light absorption measured by opalescent plate method

Aiba\textsuperscript{11} reported an opalescent plate method, which had been developed by Shibata\textsuperscript{9} for spectrophotometry of translucent biological materials, for measurement of light absorption in a microorganisms suspension. We performed measurement of light absorption in a \textit{Chlorella ellipsoidea} suspension using the apparatus shown in Fig. 3. A monochromatic parallel light beam of wavelength $\lambda$ irradiated an algae suspension. A photocell detected the intensity of a diffused light beam passed through an opalescent plate (0.5 mm thick Teflon plate) attached to the rear surface.
of a glass vessel. By this method we can obtain a distinct absorption spectrum of suspended algae.

In an algae suspension the following equation holds.

\[ I_{\alpha,\lambda} = I_{d,\lambda} + I_{L,\lambda} + I_{\text{d,}\lambda} \]  

(4)

When an infrared light beam irradiates the suspension, the equation above is rewritten as Eq. (5) since algae do not usually absorb infrared light.

\[ I_{\alpha,\lambda} = I_{d,\lambda} + I_{\text{d,}\lambda} \]  

(5)

The fraction of light absorbed by algae cells is given by the following equation.

\[ \frac{I_{\alpha,\lambda}}{I_{\text{d,}\lambda}} = 1 - \frac{I_{L,\lambda}}{I_{\text{d,}\lambda}} \left( 1 + \frac{I_{d,\lambda}}{T_{d,\lambda}} \right) \]  

(6)

If it is assumed that the ratio of dispersed visible light intensity to that transmitted is equal to one for infrared light, Eq. (6) becomes as follows:

\[ \frac{I_{\alpha,\lambda}}{I_{\text{d,}\lambda}} = 1 - \frac{T_{d,\lambda}}{T_{\alpha,\lambda}} \]  

(7)

Here \( T_{\lambda} \) and \( T_{\alpha,\lambda} \) are transmittance measured by the opalescent plate method for visible and infrared light respectively. The average absorption fraction over a certain wavelength range in which the incident light energy spectrum is expressed by \( F_{\lambda}/F_{\tau} \) becomes

\[ \bar{q} = \sum_{\lambda} \left( F_{\lambda}/F_{\tau} \right) q_{\lambda} \]  

(8)

2.2 Model parameter estimation

The two significant model parameters, \( p_f \) and \( \tau \), must be determined prior to the Monte Carlo simulation. We determined them from spectrophotometry data obtained by the opalescent plate method. We measured transmittance of the \textit{Chlorella ellipsoidea} suspension in a wavelength range from 350 nm to 720 nm, changing algae concentrations up to 0.2 volume percent. The open circles in Fig. 4 show transmittance at 720 nm for various Chlorella concentrations. As Chlorella does not absorb this infrared light, we compared these data with transmittance computed on condition that \( \tau = 1 \) and \( p_f \) took various values. From the comparison in Fig. 4 we determined that \( p_f = 0.97 \). Once \( p_f \) was determined we compared visible light transmittance with that from the random-walk simulation where \( \tau \) took various values. Figure 5 shows two examples of the comparison. At the wavelength of 560 nm Chlorella scarcely absorbs the light, then we obtained a \( \tau \) value of nearly equal one. At 680 nm Chlorella shows more absorption of the light. In Fig. 6 we show the relationship between \( \log(1/\tau_{\lambda}) \) and wavelength \( \lambda \). The solid curve is the absorbance of chloroplast\(^{10}\). The two spectra are very close, which means that the estimated values of \( \tau_{\lambda} \) are acceptable.

As the model parameters have been determined, we can now compute the light absorption fraction in an algae suspension based on the random-walk model. On the other hand, the opalescent plate method experimentally provides a light absorption fraction for a suspension with a small light path length. In
Fig. 7 the two light absorption fractions which are averaged over a wavelength range of the incident light source are compared for a Chlorella suspension with $L=1\text{ cm}$. The agreement is quite satisfactory.

2.3 Light intensity measurement by chemical actinometry

To confirm the validity of the random-walk model, we performed a chemical actinometric measurement of scattering light intensity. We used the experimental apparatus shown in Fig. 8. A parallel light beam from a tungsten lamp irradiated a cubical glass vessel filled with a Chlorella suspension. The rear face and the side of the vessel were connected with actinometer chambers filled with Reineke’s salt solution for measurement of the intensity of scattering light escaping from each face. The reaction rate of the actinometer is given by the following equations.

In the rear chamber:

$$ r_r = \frac{1}{I_{o,\lambda}} \sum \phi_{\lambda} I_{r,\lambda} (1 - e^{-\mu_{\lambda} I_{r,\lambda}}) \quad (9) $$

In the side chamber:

$$ r_s = \frac{1}{I_{o,\lambda}} \sum \phi_{\lambda} I_{s,\lambda} (1 - e^{-\mu_{\lambda} I_{s,\lambda}}) \quad (10) $$

Here, $I_{r,\lambda}$ is the intensity of light passed through the rear face of the suspension vessel and $I_{s,\lambda}$ is that through the side face. When no algae suspension is in the vessel the reaction rate in the rear actinometer chamber becomes

$$ r_r^\circ = \frac{1}{I_{o,\lambda}} \sum \phi_{\lambda} I_{o,\lambda} (1 - e^{-\mu_{\lambda} I_{o,\lambda}}) \quad (11) $$

Here, $I_{o,\lambda}$ is incident light intensity. When the following equations hold,

$$ I_{o,\lambda} = (F_{\lambda}/F_i) I_{o,\lambda} \quad (F_{\lambda}/F_i) I_{o,\lambda} $$

$$ T_{r,\lambda} = I_{r,\lambda}/I_{o,\lambda} $$

$$ T_{s,\lambda} = I_{s,\lambda}/I_{o,\lambda} $$

$$ I_o = I_{o,\lambda} $$

the ratios of the reaction rates become as follows:

$$ \frac{r_r}{r_r^\circ} = \frac{\sum \phi_{\lambda} (F_{\lambda}/F_i) T_{r,\lambda} (1 - e^{-\mu_{\lambda} I_{r,\lambda}})}{\sum \phi_{\lambda} (F_{\lambda}/F_i) (1 - e^{-\mu_{\lambda} I_{o,\lambda}})} \quad (13) $$

and

$$ \frac{r_s}{r_r^\circ} = \frac{\sum \phi_{\lambda} (F_{\lambda}/F_i) T_{s,\lambda} (1 - e^{-\mu_{\lambda} I_{s,\lambda}})}{\sum \phi_{\lambda} (F_{\lambda}/F_i) (1 - e^{-\mu_{\lambda} I_{o,\lambda}})} \quad (14) $$

In the above equations the quantum yield, $\phi_{\lambda}$, is given in the literature, and the spectrum of the incident light source and the attenuation coefficient of Reineke’s salt solution, $\mu_{\lambda}$, are determined experimentally. Furthermore, $T_{r,\lambda}$ and $T_{s,\lambda}$ can be evaluated by the random-walk model. Therefore, we can calculate the values of the right side in Eqs. (13) and (14), and compare them with the ratios of the experimental reaction rates. Figure 9 shows the results. The agreement is fairly satisfactory.

3. Discussion

From the above experimental results the proposed random-walk model has been verified to be useful for assessment of light energy absorption in an algae suspension. Figure 10 shows fractions of light energy absorbed in rectangular cultivators with a light path length of 2.5 cm, 5 cm, or 10 cm, and a $10 \times 10\text{ cm}^2$
irradiated area. The solid curves are the results computed by the random-walk model. The dotted curves are the values predicted by Lambert-Beer’s law. The difference between the two results is rather large, in particular for a long-light path cultivator. The values predicted by Lambert-Beer’s law tend toward one as \( \psi \) increases. On the other hand the solid curves by the light-scattering model converge on certain values less than one as the algae concentration becomes higher. This means that a portion of incident light escapes from the suspension because of light scattering. This energy loss takes place in a real cultivator. In particular, it becomes remarkable in one with a short light path length.

Koizumi et al.\(^6\)) also reported the same energy loss due to light scattering in the Monte Carlo method assessment of light absorption rate by \textit{Rhodopseudomonas spheroides} S cells. They pointed out that a portion of incident light energy is diffused through the side and the front surfaces of a culture vessel and that the loss becomes more pronounced for a vessel with a shorter light path length.

**Conclusion**

A new random-walk model has been proposed to assess light energy absorbed in a photosynthetic microorganism suspension. The model includes two significant parameters. One represents the light-absorbing property of a microbe cell, and is treated as a function of light wavelength. The other parameter represents the light-scattering property of the cell. These model parameters can be determined from the light transmission data measured by the opalescent plate method.

Light absorption fractions computed by the random-walk model for a \textit{Chlorella ellipsoidea} suspension were compared with experimental results obtained by the opalescent plate method. And the rates of actinometric reaction induced by scattering light escaping from the algae suspension vessel were experimentally measured and compared with the values predicted by the random-walk model. The agreement was satisfactory. The proposed random-walk model can properly assess light energy absorption by a photosynthetic microorganism.

**Nomenclature**

- \( d \) = diameter of microbe cell [m]
- \( F_0/F_i \) = incident light energy spectrum [–]
- \( I_0 \) = background scattering light intensity [J·m\(^{-2}\)·s\(^{-1}\)·•]
- \( I_s \) = forward scattering light intensity [J·m\(^{-2}\)·s\(^{-1}\)·•]
- \( I_{s,a} \) = absorbed light intensity [J·m\(^{-2}\)·s\(^{-1}\)·•]
- \( I_{s,a} \) = total incident light intensity [J·m\(^{-2}\)·s\(^{-1}\)·•]
- \( I_{s,a} \) = incident light intensity [J·m\(^{-2}\)·s\(^{-1}\)·•]
- \( I_{s,a} \) = light intensity passed through side face of suspension vessel [J·m\(^{-2}\)·s\(^{-1}\)·•]
- \( I_{s,a} \) = transmitted light intensity [J·m\(^{-2}\)·s\(^{-1}\)·•]
- \( l_i \) = side length of unit block [m]
- \( l_m \) = side length of subunit [m]
- \( l_0 \) = light path length in rear actinometer chamber with no suspension [m]
- \( l_i \) = average light path length in side actinometer chamber [m]
- \( P_s \) = backward-escaping probability [–]
- \( P_f \) = forward-escaping probability [–]
- \( P_s \) = side-ward-escaping probability [–]
- \( \rho_f \) = probability of forward scattering [–]
- \( \rho_s \) = probability of hit, given by Eq. (3) [–]
- \( \rho_s \) = probability of side-ward scattering [–]
- \( q_{s,a} \) = light absorption fraction [–]
- \( r_s \) = wavelength average absorption fraction [–]
- \( r_i \) = reaction rate of the Reinecke’s salt actinometer in side chamber [mol·m\(^{-3}\)·s\(^{-1}\)·•]
- \( r_s \) = reaction rate of the Reinecke’s salt actinometer in rear chamber [mol·m\(^{-3}\)·s\(^{-1}\)·•]
- \( T_{s,a} \) = \( I_{s,a}/I_0 \) [–]
- \( T_{s,a} \) = \( I_{s,a}/I_0 \) [–]
- \( T_e \) = transmittance measured by opalescent plate method [–]
- \( V \) = suspension volume [m\(^3\)·•]
- \( \lambda \) = wavelength of light [nm]
- \( \mu_s \) = attenuation coefficient of Reinecke’s salt solution [m\(^{-1}\)·•]
- \( \mu_s \) = light intensity decrease parameter [–]
- \( \phi_s \) = quantum yield of Reinecke’s salt actinometer [mol·J\(^{-1}\)·•]
- \( \psi \) = volume fraction of microbe in suspension [–]
- \( \times \) = denote quantity for infrared light

**Literature Cited**


