photonics

MDPI

Supplementary Materials

1. Composion of BG11 medium

Table S1. BG11 (Blue-Green Medium) [1]

#	Component	Concentration
1	$NaNO_3$	1.5 g/L
2	K_2HPO_4	0.04 g/L
3	$MgSO_4{\cdot}7H_2O$	0.075 g/L
4	$CaCl_2{\cdot}2H_2O$	0.036 g/L
5	Citric acid	0.006 g/L
6	Ferric ammonium citrate	0.006 g/L
7	$EDTANa_2$	0.001 g/L
8	Na_2CO_3	0.02 g/L
9	A5 (Trace mental solution)*	1 ml/L

Table S2. A5 (Trace mental solution)*

#	Component	Concentration
1	H_3BO_3	2.86 g/L
2	$MnCl_2{\cdot}4H_2O$	1.86 g/L
3	$ZnSO_4{\cdot}7H_2O$	0.22 g/L
4	$Na_2MoO_4{\cdot}2H_2O$	0.39 g/L
5	$CuSO_4{\cdot}5H_2O$	0.08 g/L
6	$Co(NO_3)_2{\cdot}6H_2O$	0.05 g/L

2. The effective spectral absorption and scattering coefficients κ_λ and $\sigma_{s,\lambda}$, H-G phase function Φ_{HG} and average single scattering albedo ω_{eff}

The expressions of κ_λ, $\sigma_{s,\lambda}$ and Φ_{HG} are written as [2]

$$\kappa_\lambda = \kappa_{L,\lambda}(1 - f_b - X_a \upsilon_{Xa}) + A_{abs,\lambda} X_a , \quad (1)$$

$$\sigma_{s,\lambda} = \sigma_{Xa,\lambda} + \sigma_{b,\lambda} = S_{sca,\lambda} X_a + (A_b / 4) Q_{sca,b} , \quad (2)$$

$$\Phi_{HG,i}(\theta) = \frac{1 - g_i^2}{(1 + g_i^2 - 2 g_i \cos\theta)^{3/2}}, \quad i = X_a \text{ or } b , \quad (3)$$

$$\Phi_{HG,\lambda}(\theta) = \frac{\sigma_{b,\lambda}\Phi_{HG,b}(\theta) + \sigma_{Xa,\lambda}\Phi_{HG,Xa}(\theta)}{\sigma_{s,\lambda}}, \quad (4)$$

where $\kappa_{L,\lambda}$ is the absorption coefficient of the liquid phase (m^{-1}). X_a is the concentration of microalgae (kg/m^3). $A_{abs,\lambda}$ is the mass absorption cross-section of microalgae (m^2/kg). υ_{Xa} is the specific volume of microalgae (generally 0.001 m^3/kg). $S_{sca,\lambda}$ is the mass scattering cross-section of microalgae (m^2/kg). f_b is the volume fraction of bubbles (usually $0 \le f_b \le 0.3$). $Q_{sca,b}$ is the scattering efficiency factor of bubbles. g_i is the asymmetry factor of microalgae or bubbles. The interfacial area concentration A_b is expressed as $A_b = 3f_b/a$ (m^{-1}). a is bubble radius (m). $\Phi_{HG,\lambda}$ is the total scattering phase function.

The scattering efficiency factor $Q_{sca,b}$ and the scattering phase function of the bubbles Φ_b are predicted by Mie theory [3] applied to a sphere of radius a (3.5 μm, 35 μm, 350 μm, 3.5 mm) and refractive index 1 embedded in water with $n_L = 1.33$. The results indicate that $Q_{sca,b}$ is equal to 1.0 (corrected for the diffraction paradox) and it generally varies less than

0.1% (a = 3.5 mm), 0.2% (a = 350 μm), 0.5% (a = 35 μm), 5% (a = 3.5 μm) in the considering spectrum. Similarly, it was found that Φ_b is strongly forward and does not vary appreciably for the size parameters considered. The asymmetry factors g_b are 0.84600 (a = 3.5 mm, deviation < 0.04%), 0.84613 (a = 350 μm, deviation < 0.2%), 0.85087 (a = 35 μm, deviation < 0.5%), and 0.85597 (a = 3.5 μm, deviation < 1.5%) in the considering spectrum. In order to simplify the calculations, the phase function of the bubble is approximated as H-G phase function with g_b obtained by Mie theory.

In addition, the average single scattering albedo ω_{eff} over N boxes of the spectrum is used to assess the overall contribution of the scattering to extinction and is calculated as [2]

$$\omega_{\text{eff}} = \frac{\sum_i^N \sigma_{s,\lambda}}{\sum_i^N (\sigma_{s,\lambda} + \kappa_\lambda)}. \quad (5)$$

3. Light source and boundary reflection

The irradiance on the outer surface of the PBR is measured by an optical power and energy meter (model PM100D, Thorlabs, USA) and is shown in Figure S1 It is assumed that all the light emitted by LED lamps is diffusely incident on the surface of the PBR. The reflection and transmission of the inner and out surface of the PBR are taken into consideration, while the absorption of the PBR wall is negligible, and the light reflected by LED lamp again reaches the PBR is also omitted. Then the effective incident irradiance G_{in} is defined as the irradiance of incident light transferring through the wall to the surface of microalgal culture, and is expressed as [4,5]

$$G_{\text{in}} = E_{\text{LED}} \frac{T_{01}T_{12}}{1 - R_{10}R_{12}}, \quad (6)$$

where E_{LED} is the irradiance of LED lights, obtained form Figure S1 by integration. T_{ij} and R_{ij} are the diffuse reflectance and transmittance at the interface between two neighboring media (incident from i to j), and 0 represents air, 1 represents PBR wall, and 2 represents microalgal culture. The diffuse reflectance and transmittance of the interface are written as [6]

$$R = 2\int_{\theta=0}^{\theta=\pi/2} \rho(\theta)\sin(\theta)\cos(\theta)\,d\theta, \quad T = 1 - R, \quad (7)$$

where $\rho(\theta)$ is the specular reflectivity of the interface at incident angle θ according to Fresnel reflection. The wall reflectance R_w, i.e. the boundary condition, when lights illuminate the inner surface of the PBR from the inside to the outside, is defined as [4]

$$R_w = R_{21} + \frac{T_{21}T_{12}R_{10}}{1 - R_{12}R_{10}}, \quad (8)$$

The optical constant of PMMA is obtained from Ref. [7]

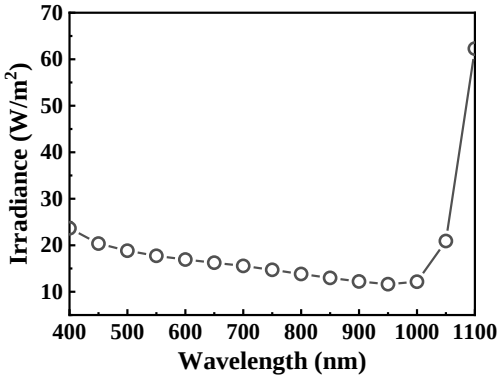

Figure S1. The spectral irradiance of LED lights.

4. The transmitted light intensity for *S. obliquus*

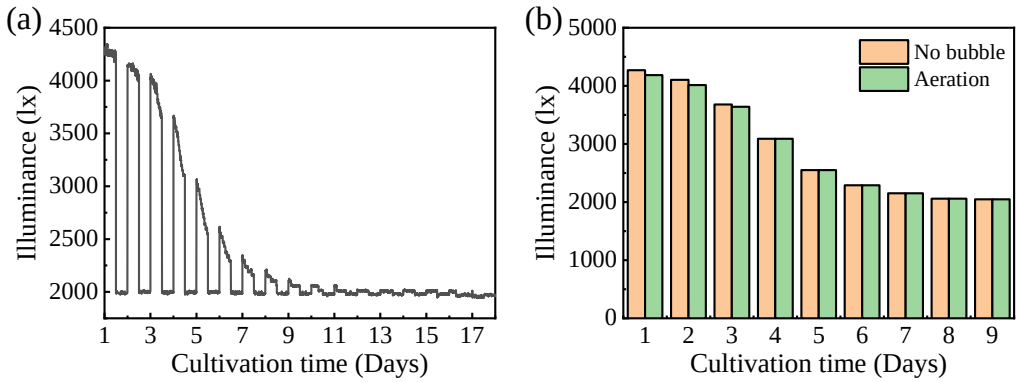

Figure S2. (a) The transmitted light intensity of the PBR of *S. obliquus* with respect to cultivation days. (b) The transmitted light intensity of the PBR with and without aeration every day.

5. Summary of the optical properties of microalgae and boundary conditions in box model

The time-dependent radiation characteristics of microalgae as well as optical properties of liquid phase and bubbles are approximated with the box model, as summarized in Table S3 and Figure S3. Boxes 1 and 3 capture the absorption peaks of the pigment which is responsible for providing energy for photosynthesis. The scattering efficiency factor of bubbles is equal to 1 corrected for the diffraction paradox, and other parameters' values are as follows: bubble radius a = 3.5 mm and retention time = 2.3 s (obtained from software analysis of photographs), aeration rate = 2 L/min, total culture volume = 24.6 L, optical path L = 0.08 m. Then bubble volume fraction f_b = 0.003 and interfacial area concentration A_b = 2.66 m^{-1} are obtained through simple arithmetic.

Table S3. Summary of the optical properties of *Chlorella* sp. on day 13 and boundary conditions in box model.

Spectrum	λ (nm)	400-520	520-630	630-720	720-1100
Liquid phase	$\kappa_{L,\lambda} \times 10^3$ (m^{-1})	28.02	129.80	507.05	15255.63
Bubble	$Q_{sca,b}$	1.0	1.0	1.0	1.0
	g_b	0.8460	0.8460	0.8460	0.8460
Microalga	$A_{abs,\lambda}$ ($m^2 \cdot kg^{-1}$)	378.60	145.32	260.83	38.52
	$S_{sca,\lambda}$ ($m^2 \cdot kg^{-1}$)	1550.7	1920.5	1604.8	1443.9
	g_{Xa}	0.98	0.98	0.98	0.98
Effective incident irradiance	$G_{in,\lambda}$ ($W \cdot m^{-2}$)	1969.20	1543.22	1157.43	5009.77
Boundary reflectance	R_w	0.5346	0.5311	0.5292	0.5181

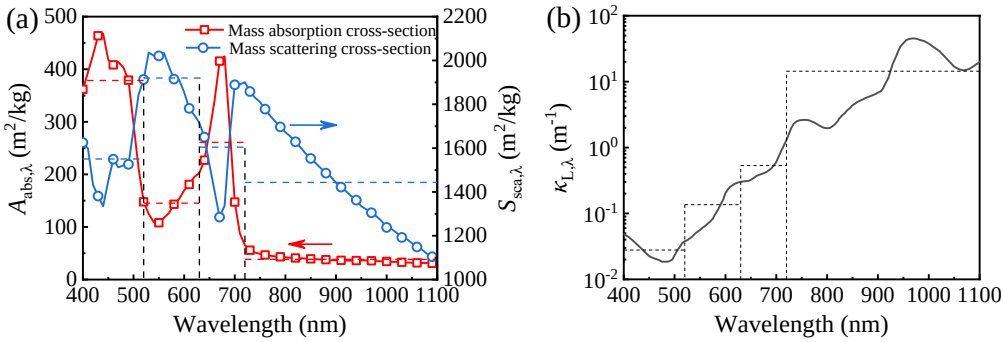

Figure S3. (a) The spectral mass scattering and absorption cross-sections of *Chlorella* sp. on day 13. (b) The spectral absorption coefficient of water.

6. Method of solution

The finite volume method (FVM) was employed to discretely solve the RTE (see mathematical details in Refs.[8,9]), assuming that the light transfer is one-dimensional. It consists of transforming a hyperbolic partial differential equation into a set of ordinary differential equations. The one-dimensional grid is composed of 1200 points. The integral for the in-scattering term is computed with two Gauss quadrature having 24 discrete directions per hemisphere. Then, the ordinary differential equations are solved using the fourth order Runge–Kutta method at every point. Finally, the local spectral irradiance is defined as

$$G_\lambda(x) = \int_{4\pi} I_\lambda(x,\hat{s})\mathrm{d}\Omega = 2\pi \sum_{i=1}^{24} w_i I_\lambda(x,\theta_i), \quad (9)$$

where w_i is the weighting factor. The local spectral irradiance calculated for each of the four boxes are added to give the total local irradiance as

$$G(x) = G_{400-520}(x) + G_{520-630}(x) + G_{630-720}(x) + G_{720-1100}(x), \quad (10)$$

7. Temporal evolutions of average single scattering albedo for microalgal cultures

Figure S4 shows the temporal evolutions of average single scattering albedo of *Chlorella* sp. and *S. obliquus*, which indicated that the average albedo increased due to the microalgal cell density increased with growth time. Besides incident light, there was scattering light of the microalgae and bubbles illuminated back on the culture surface, coupled with boundary reflection. Therefore the irradiance on the illuminated surface was enhanced, which may be larger than the incident irradiance and the normalized local irradiance larger than 1 occurs.

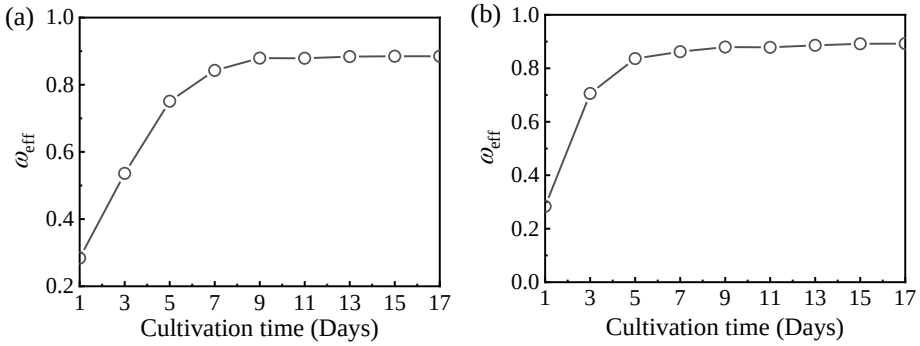

Figure S4. Temporal evolutions of average single scattering albedo of (a) *Chlorella* sp. and (b) *S. obliquus*.

8. Specific growth rate modelling

The specific growth rate μ, defined by $dN/dt=\mu N$ (N is cell density) and expressed in d^{-1}, has been modeled using the Haldane model taking into account light saturation and inhibition as [10]

$$\mu=\mu_{max}\frac{G}{K_s+G+G^2/K_i}, \tag{11}$$

where G denotes the available irradiance, μ_{max} is the maximum specific growth rate, and the coefficients K_s and K_i are the light half-saturation and inhibition constants respectively.

The average specific growth rate $\langle\mu\rangle$ calculated all over the PBR is obtained by integrating local growth rate. Due to the one-dimensional radiation distribution of the PBR, integration is reduced to the distance x from the illuminated culture surface along the thickness L, which gives

$$\langle\mu\rangle=\frac{1}{L}\int_0^L \mu dx, \tag{12}$$

Identification of the model parameters has been achieved by least-squares fitting with the experimental data of Ref. [11]. The results are shown in Figure S5 and give μ_{max} = 2.944 d^{-1}, K_s = 1813 lx, K_i = 19580 lx for *Chlorella* sp. and μ_{max} = 3.098 d^{-1}, K_s = 4448 lx, K_i = 21060 lx for *S. obliquus*. And the local specific growth rates for different bubble parameters are shown in Figure S6.

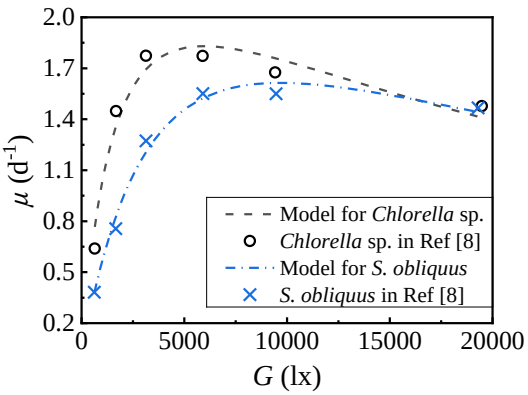

Figure S5. Specific growth rates of experimental data and kinetic model fitting with different irradiance.

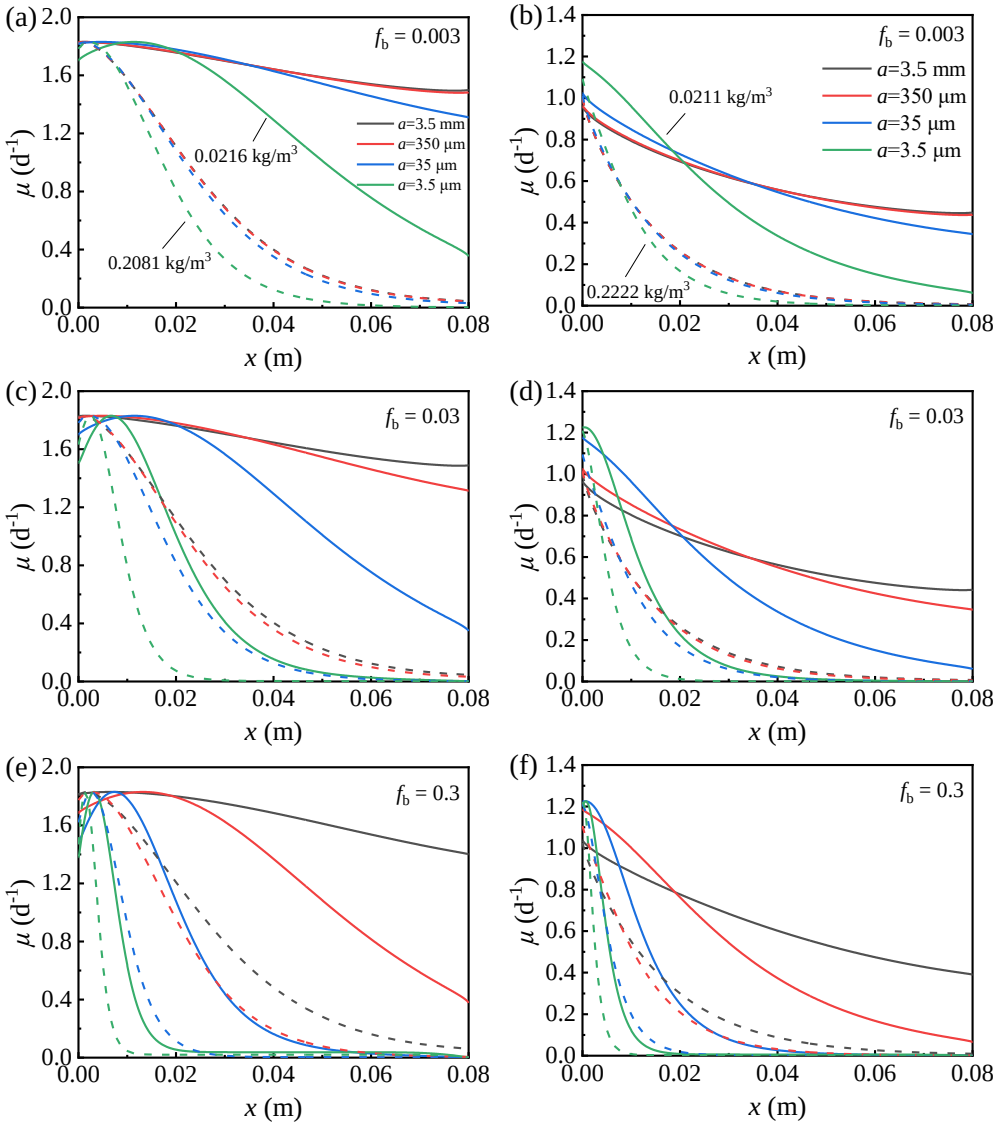

Figure S6. Local specific growth rates for different bubble volume fraction and radius of (a,c,e) *Chlorella* sp. and (b,d,f) *S. obliquus*. (Solid lines: low microalgae concentration. Dashed lines: high microalgae concentrations.)

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