Supplementary Material for Photosynthesis Research article: Cost and color of photosynthesis

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Photosynthetic growth power optimization

Question:

What spectral distribution would optimize P_{G} if the organism could freely tune the resonance frequency of the electronic transition dipoles that make up its absorption spectrum and the energy it invests in equipment for chemical storage of the absorbed power.

Strategy:

1. Express P_{G} in terms of the absorber distribution by dividing the relevant part of the spectrum into n sufficiently small frequency steps with index i and assigning a quantity of d_i proportional to the total dipole-strength at the corresponding resonance frequency. The optimum for P_{G} is then found by setting its gradient to zero, i.e. equating the partial derivatives of P_{G} with respect to all d_i to zero, and solving the resulting n equations, $\{{}^{\partial P_{\mathrm{G}}}/_{\partial d_i}\}_{i=1..n} = 0$.

2. Express P_{G} in terms of P_{sat}. The optimal investment in the equipment for chemical storage is then found by solving ${}^{\partial \mathrm{P_G}}/_{\partial \mathrm{P_{sat}}} = 0$.

By substituting the results of the latter optimization into the former, the condition for optimal P_{G} is found.

Optimization of investment in light-harvesting equipment

Using $P_{\mathrm{G}} = P_{\mathrm{out}} \cdot C_{\mathrm{G}}$ we have:

$$\frac{\partial P_{\mathrm{G}}}{\partial d_i} = \frac{\partial P_{\mathrm{out}}}{\partial d_i} \cdot C_{\mathrm{G}} + P_{\mathrm{out}} \cdot \frac{\partial C_{\mathrm{G}}}{\partial d_i} = 0$$

$$\Rightarrow$$

$$\frac{\partial P_{\mathrm{out}}}{\partial d_i} = -P_{\mathrm{out}} \cdot \frac{1}{C_{\mathrm{G}}} \frac{\partial C_{\mathrm{G}}}{\partial d_i} \tag{1}$$

C_{G} is the *relative* amount of energy that is not spent on reproduction of the growth generating equipment. By defining E_{G} as the corresponding *absolute* amount and E_{tot} the total amount of energy spent on the organism,

$$C_{\mathrm{G}} = \frac{E_{\mathrm{G}}}{E_{\mathrm{tot}}}$$

Assuming that one term of E_{tot}, the energy spent on light-harvesting E_{LH}, is proportional to $D = \sum d$, i.e.

$$\frac{\partial E_{\mathrm{LH}}}{\partial d_i} = \frac{E_{\mathrm{LH}}}{D}$$

we have:

$$\frac{\partial C_{\mathrm{G}}}{\partial d_i} = -\frac{E_{\mathrm{LH}}}{D} \cdot \frac{E_{\mathrm{G}}}{E_{\mathrm{tot}}^2}$$

and therefore:

$$\frac{1}{C_{\mathrm{G}}}\frac{\partial C_{\mathrm{G}}}{\partial d_i} = -\frac{1}{D} \cdot \frac{E_{\mathrm{LH}}}{E_{\mathrm{tot}}} \equiv -\frac{1}{D} \cdot C_{\mathrm{Pin}}$$

and thus by substituting into (1):

$$\frac{\partial P_{\mathrm{out}}}{\partial d_i} = P_{\mathrm{out}} \cdot \frac{C_{\mathrm{Pin}}}{D} \tag{2}$$

With $P_{\mathrm{out}} = 1/\left(1/P_{\mathrm{in}} + 1/P_{\mathrm{sat}}\right)$

$$\begin{aligned}\frac{\partial P_{\mathrm{out}}}{\partial d_i} &= \frac{\partial P_{\mathrm{out}}}{\partial P_{\mathrm{in}}} \cdot \frac{\partial P_{\mathrm{in}}}{\partial d_i} \\ &= \left(1 + \frac{P_{\mathrm{in}}}{P_{\mathrm{sat}}}\right)^{-2} \cdot \frac{\partial P_{\mathrm{in}}}{\partial d_i}\end{aligned}$$

and by substituting this into (2):

$$\frac{\partial P_{\mathrm{in}}}{\partial d_i} = \left(1 + \frac{P_{\mathrm{in}}}{P_{\mathrm{sat}}}\right) \cdot P_{\mathrm{in}} \cdot \frac{C_{\mathrm{Pin}}}{D} \tag{3}$$

From the equation for the input power the partial derivative of P_{in} can be evaluated as follows:

$$\begin{aligned}\frac{\partial P_{\mathrm{in}}}{\partial d_i} &= \frac{\partial J_{\mathrm{L}}}{\partial d_i} \cdot \mu + J_{\mathrm{L}} \cdot \frac{\partial \mu}{\partial d_i} \\ &= \frac{\partial J_{\mathrm{L}}}{\partial d_i} \cdot \mu + kT \cdot J_{\mathrm{L}} \cdot \left(\frac{\partial J_{\mathrm{L}}/\partial d_i}{J_{\mathrm{L}}} - \frac{\partial J_{\mathrm{D}}/\partial d_i}{J_{\mathrm{D}}}\right) \\ &= \frac{\partial J_{\mathrm{L}}}{\partial d_i}\left(\mu + kT\right) - kT \cdot \left(\frac{J_{\mathrm{L}}}{J_{\mathrm{D}}}\frac{\partial J_{\mathrm{D}}}{\partial d_i}\right) \\ &= \frac{\partial J_{\mathrm{L}}}{\partial d_i}\left(\mu + kT\right) - kT \cdot \left(e^{\mu/kT} \cdot \frac{\partial J_{\mathrm{D}}}{\partial d_i}\right)\end{aligned} \tag{4}$$

which can be evaluated further by expressing J_L and J_D as functions of d_i. This is achieved by relating the absorption cross-section to d:

$$\sigma_i = g_i \cdot h\nu_i \cdot B/c = d_i \cdot h\nu_i$$

yielding:

$$\begin{aligned}\frac{\partial J_\mathrm{L}}{\partial d_i} &= \frac{\partial}{\partial d_i}\left[\sum_{i=1}^{n} I_{\mathrm{sol},i}\left(1 - e^{-\sigma_i}\right)\right] \\ &= I_{\mathrm{sol},i} \cdot \frac{\partial \sigma_i}{\partial d_i} \cdot e^{-\sigma_i} \\ &= I_{\mathrm{sol},i} \cdot h\nu_i \cdot e^{-\sigma_i}\end{aligned}$$

and

$$\begin{aligned}\frac{\partial J_\mathrm{D}}{\partial d_i} &= \frac{\partial}{\partial d_i}\left[\sum_{i=1}^{n} \sigma_i \cdot I_{\mathrm{bb},i}\right] \\ &= \frac{\partial \sigma_i}{\partial d_i} \cdot I_{\mathrm{bb},i} \\ &= h\nu_i \cdot I_{\mathrm{bb},i}\end{aligned}$$

Substituting these in (4) gives:

$$\frac{\partial P_\mathrm{in}}{\partial d_i} = I_{\mathrm{sol},i} \cdot h\nu_i \cdot e^{-\sigma_i}\left(\mu + kT\right) - kT \cdot \left(e^{\mu/kT} \cdot I_{\mathrm{bb},i} \cdot h\nu_i\right)$$

Substituting this expression on the left-hand side of (3) yields the n equations that determine the d_i that optimize the growth power:

$$I_{\mathrm{sol},i} \cdot h\nu_i \cdot e^{-\sigma_i}\left(\mu + kT\right) - kT \cdot \left(e^{\mu/kT} \cdot I_{\mathrm{bb},i} \cdot h\nu_i\right) = \left(1 + \frac{P_\mathrm{in}}{P_\mathrm{sat}}\right) \cdot P_\mathrm{in} \cdot \frac{C_\mathrm{Pin}}{D}$$

$$\Rightarrow$$

$$I_{\mathrm{sol},i} \cdot h\nu_i \cdot e^{-\sigma_i} = \frac{1}{\mu + kT} \cdot \left[kT \cdot e^{\mu/kT} \cdot I_{\mathrm{bb},i} \cdot h\nu_i + \left(1 + \frac{P_\mathrm{in}}{P_\mathrm{sat}}\right) \cdot P_\mathrm{in} \cdot \frac{C_\mathrm{Pin}}{D}\right] \tag{5}$$

Optimization of investment in the equipment for chemical storage of the absorbed power

We assume that the amount of energy spent on the chemical storage machinery is a term in E_tot , designated E_chem which is proportional to the saturation power P_sat:

$$\frac{dE_\mathrm{chem}}{dP_\mathrm{sat}} = \frac{E_\mathrm{chem}}{P_\mathrm{sat}}$$

The optimization of P_G in terms of the d_i must be extended to the requirement that

$$\frac{dP_\mathrm{G}}{dP_\mathrm{sat}} = 0$$

as well, i.e.,

$$\begin{aligned}\frac{dP_{\mathrm{G}}}{dP_{\mathrm{sat}}} &= \frac{dP_{\mathrm{out}}}{dP_{\mathrm{sat}}}C_{\mathrm{G}} + P_{\mathrm{out}}\frac{dC_{\mathrm{G}}}{dP_{\mathrm{sat}}} \\ &= -\frac{P_{\mathrm{out}}^2}{P_{\mathrm{sat}}^2}C_{\mathrm{G}} + P_{\mathrm{out}} \cdot \frac{E_{\mathrm{G}} \cdot {}^{dE_{\mathrm{chem}}}\!/\!{}_{dP_{\mathrm{sat}}}}{E_{\mathrm{tot}}^2} \\ &= -\frac{P_{\mathrm{out}}^2}{P_{\mathrm{sat}}^2}C_{\mathrm{G}} + P_{\mathrm{out}} \cdot C_{\mathrm{G}} \cdot \frac{E_{\mathrm{chem}}}{E_{\mathrm{tot}}P_{\mathrm{sat}}} \\ &= -\frac{P_{\mathrm{out}}^2}{P_{\mathrm{sat}}^2}C_{\mathrm{G}} + P_{\mathrm{out}} \cdot C_{\mathrm{G}} \cdot \frac{C_{\mathrm{Pout}}}{P_{\mathrm{sat}}} \\ &= 0\end{aligned}$$

from which we have:

$$\begin{aligned}\frac{P_{\mathrm{out}}^2}{P_{\mathrm{sat}}^2} &= P_{\mathrm{out}} \cdot \frac{C_{\mathrm{Pout}}}{P_{\mathrm{sat}}} \Rightarrow \\ \frac{P_{\mathrm{out}}}{P_{\mathrm{sat}}} &= C_{\mathrm{Pout}}\end{aligned} \tag{6}$$

With $P_{\mathrm{out}} = 1/\left(1/P_{\mathrm{in}} + 1/P_{\mathrm{sat}}\right)$ substituted into (6) we get:

$$\begin{aligned}\frac{P_{\mathrm{in}}/P_{\mathrm{sat}}}{1 + P_{\mathrm{in}}/P_{\mathrm{sat}}} &= C_{\mathrm{Pout}} \\ &\Rightarrow \\ \frac{1}{1 + P_{\mathrm{in}}/P_{\mathrm{sat}}} &= 1 - C_{\mathrm{Pout}} \\ &= C_{\mathrm{Pin}} + C_{\mathrm{G}}\end{aligned}$$

which can be substituted into (5) giving the condition for optimal P_{G}:

$$I_{\mathrm{sol},i} \cdot h\nu_i \cdot e^{-\sigma_i} = \frac{1}{\mu + kT} \cdot \left[kT \cdot e^{\mu/kT} \cdot I_{\mathrm{bb},i} \cdot h\nu_i + P_{\mathrm{in}} \cdot \frac{C_{\mathrm{Pin}}}{\left(C_{\mathrm{Pin}} + C_{\mathrm{G}}\right)D}\right] \tag{7}$$

Solving numerically

Treating the indexed quantities as vectors,

$$\begin{aligned}\vec{T}_i &= I_{\mathrm{sol},i} \cdot h\nu_i \cdot e^{-\sigma_i} \\ \vec{B}_i &= I_{\mathrm{bb},i} \cdot h\nu_i\end{aligned}$$

and by designating the non-indexed quantities:

$$\begin{aligned}f\left(\vec{T}\right) &\equiv \frac{kT}{\mu + kT} \cdot e^{\mu/kT} \\ g\left(\vec{T}, C\right) &\equiv \frac{1}{\mu + kT} \cdot \frac{P_{\mathrm{in}}}{D} \cdot \frac{C_{\mathrm{Pin}}}{\left(C_{\mathrm{Pin}} + C_{\mathrm{G}}\right)}\end{aligned}$$

equation (7) becomes:

$$\vec{T} = f\left(\vec{T}\right)\vec{B} + g\left(\vec{T}, C\right)\vec{u} \tag{8}$$

where $\vec{u}$ is a vector containing (n) ones. While $\vec{B}$ and $\vec{u}$ are known, the vectors $\vec{T}^m$ must be found that satisfy (8) in the range $0 \leq C \leq 1$.

Equation (8) is a fixed point equation and is solved by iterative mapping, starting with an initial guess for $\vec{T} = \vec{T}^0$:

$$\begin{aligned} \vec{T}^1 &\rightarrow f\left(\vec{T}^0\right)\vec{B} + g\left(\vec{T}^0, C\right)\vec{u} \\ \vec{T}^2 &\rightarrow f\left(\vec{T}^1\right)\vec{B} + g\left(\vec{T}^1, C\right)\vec{u} \\ \vdots &\rightarrow \vdots \end{aligned}$$

until the iterations converge to $\vec{T}^*$:

$$\vec{T}^* = f\left(\vec{T}^*\right)\vec{B} + g\left(\vec{T}^*, C\right)\vec{u}$$

If a (smooth) 5800 K black-body curve is used to simulate I_{sol} the iterative map gives a unique solution irrespective of $\vec{T}^0$ for all *C*. With the actual I_{sol} at sea level, however, local extrema may prevent the iteration from converging to the optimum for very low and very high C and $\vec{T}^0$ must be scanned over a suitable range.