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Analytical model of ion transport and conversion of light energy in chloroplasts

Alexey V. Melkikh *, Vladimir D. Seleznev, Oksana I. Chesnokova

Ural State Technical University, 19 Mira St., 620002 Ekaterinburg, Russia

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ABSTRACT

An analytical model, which describes the stationary transformation of light energy to the energy of pigment electronic excitation, has been constructed. A proton pump of the thylakoid membrane has been considered as a two-level conformon. The difference between the energies of the excited and ground states of both the pigment and the protein complex is assumed to be the energy of an absorbed photon. It has been found how the concentration of ions in a lumen and the potential across the thylakoid membrane depend on the concentration of ions in the stroma and the brightness temperature of absorbed radiation. Conditions for the maximum efficiency of the photosynthesis process have been analyzed. This model has been used to determine the electric potential ($\varphi \approx 6.7$ mV) at the chloroplast thylakoid membrane. The calculated value of the electric potential is in good agreement with the experimental data. A limitation on the stoichiometric coefficient of the proton transport through ATP-synthase, $m > 3$, has been found theoretically.

0. Introduction

Photosynthesis in the chloroplasts of plants is of fundamental importance for the existence of biosystems on the Earth. Chloroplasts are shaped like a convexo-convex lens, 4–10 μm in diameter and 1 μm thick. The outer membrane separates the chloroplast from the rest of cytoplasm. The chloroplast wall consists of two membranes, which bind structureless contents called a stroma. The stroma is penetrated by a system of parallel elementary membranes, thylakoids, which are an extension of the inner membrane. The double membranes of the thylakoids, which are about 0.3 μm in diameter are tight against one another to form chlorophyll-containing piles or grans.

The photosynthesis process begins at the moment the chloroplast is exposed to visible light. Photosynthesis allows complex organic substances, which are necessary to implement vital functions, to be formed from simple compounds such as carbon dioxide and water. Higher plants, algae and photosynthetic bacteria carry out this process through the light energy absorbed by chlorophyll and other photosynthetic pigments. It is one of the most important biological processes, which is persistent and abundant on our planet.

Therefore, chain reactions of photosynthesis have comprehensively been studied in experiments (Nicholls, 1982; Hall and Rao, 1981; Creighton, 1999; Fleischman, 2001; Rubin, 1987). Many papers deal with theoretical models (Vershubskii et al., 2004; Riznichenko et al., 1999; Zhu et al., 2007), including a thermodynamic analysis (Jennings et al., 2005, 2006; Lavergne, 2006; Knox and Parson, 2007; Albarrán-Zavala and Angulo-Brown, 2007; Ross and Calvin, 1967; Meszena and Westerhoff, 1999; Parson, 1978) of these processes. The active proton transport through the thylakoid membrane, which is induced by absorption of photons, is an important stage of photosynthesis. However, despite a large number of theoretical studies, this problem has been addressed little. The gradient of the electrochemical potentials of protons is the exact motive force of the ATP synthesis in chloroplasts. Therefore, this significant stage of photosynthesis can hardly be overestimated.

At present, several models of photosynthesis are available (Vershubskii et al., 2004; Riznichenko et al., 1999; Zhu et al., 2007). The model by Riznichenko et al. (1999), describes in detail, the nonstationary changes in the states of the photosystem II. This allows analyzing the fluorescence as a function of time upon exposure to light. Unfortunately, light absorption has not been described explicitly. Therefore, the stationary value of the electric potential as a function of the absorbed light characteristics cannot be determined from this model. One more model (Zhu et al., 2007) describes changes in the concentration of each metabolite allowing the analysis of the photosynthesis process in terms of its efficiency. Therefore, it permits us to understand how the environmental conditions need to be changed for plants to maximize the output of certain reaction products. Unfortunately, these models do not contain equations for ion flows and cannot be used for calculating the electric potential at the membrane.

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* Corresponding author. Fax: +7 343 374 78 54.
E-mail address: melkikh2008@rambler.ru (A.V. Melkikh).

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Nomenclature

A (A_1, A_2)	radiation constant of excited molecules-conformons (K1, K2)
$\vec{c}$,c	photon velocity vector and modulus
e	electron charge
$f_{\nu\Omega}$	volume density of mode quanta $(\nu,\vec{\Omega})$
h	the Planck's constant
J_e	flow of electrons through the thylakoid membrane
J_{H}, $J_{\mathrm{H}}^{\mathrm{ATP}}$	flows of protons through the thylakoid membrane, which are due to the photosystem II and which cause the ATP synthesis, respectively
k	the Boltzmann constant
$k_{\uparrow}(k_{1\uparrow},k_{2\uparrow})$	excitation rate constants of molecules-conformons (K1, K2)
$k_{\downarrow}(k_{1\downarrow},k_{2\downarrow})$	the rate constant of transition to the ground state of molecules-conformons (K1, K2)
$k_{\mathrm{H}\uparrow}$,$k_{\mathrm{H}\downarrow}$	the rate constant of sorption and desorption of H^+ ions
$k_{\mathrm{H}}^{\mathrm{ATP}}$	the rate constant of trapping of protons by the ATP-synthase
L	distance between the Sun and the Earth
m	number of protons carried by the ATP-synthase in a single event of a synthesis reaction
M	the chlorophyll molecular weight
n^* (n_1^*, n_2^*), n^a (n_1^a,n_2^a)	density of molecules-conformons (K1, K2) in the excited and ground states, respectively
n_o^* (n_{1o}^* n_{2o}^*), n_o^a (n_{1o}^a n_{2o}^a)	equilibrium density of molecules-conformons (K1, K2) in the excited and ground states, respectively
n_2	density of molecules-conformons K2
n_i^{in}, n_{K}^{in}, n_{Cl}^{in}, n_A^{in}, n_{H}^{in}	density of ions of the ith species, potassium, chlorine, other anions, and protons in a lumen, respectively
n_i^{out}, n_{K}^{out}, n_{Cl}^{out}, n_A^{out}, n_{H}^{out}	density of ions of the ith species, potassium, chlorine, other anions, and protons in the stroma, respectively;
n_x^* (n_{xo}^*), n_x^a (n_{xo}^a)	density of ionized and nonionized chlorophyll molecules (in equilibrium), respectively
${n_x}^c$	molar concentration of the chlorophyll in a cell
n_x	average concentration of the chlorophyll in grans
$n_{\nu\Omega}$	number of photons per mode $(\nu,\vec{\Omega})$
ΔpH	difference of pH across the membrane
Q	the reaction heat
$\vec{r}$	a spatial coordinate
R_s	radius of the Sun
t	time
T, $T_{\nu\Omega}$	temperature of the thermostat and the photon mode $(\nu,\vec{\Omega})$ (the brightness radiation temperature), respectively
z_i	charge of the ith species of ions
β	average volume fraction of grans in a vegetative cell
$\Delta\mu$ ($\Delta\mu_1$, $\Delta\mu_2$)	difference between the chemical potentials of the excited and ground states of a conformon (K1, K2)
$\Delta\mu_A$	difference between the chemical potentials of the ATP hydrolysis reaction
$\Delta\mu_{\mathrm{H}}^e$	difference between the electrochemical potentials of hydrogen ions at the membrane
ν	radiation frequency
ν_{ATP}	frequency of the ATP synthesis reaction events
ξ	the efficiency of converting the photon energy to the free energy of molecules-conformons
$\sigma(\overline{\sigma} = \int d\nu\sigma(\nu))$	the (integral) interaction cross-section of photons and a molecule-conformon
φ	the electric potential at a biomembrane
$\vec{\Omega}$	a unit vector of the photon velocity

Vershubskii et al. (2004) developed a model for the electron and proton transports through the thylakoid membrane, which are connected with ATP synthesis in chloroplasts. He placed special emphasis on the lateral transport of ions and electron carrier molecules. He then compared his results with experimental data on the lateral diffusion of protons in the thylakoid gap. Formulas for the passive flow of protons and their flow in the ATP-synthase were adduced. However, mathematical modeling of the flow of hydrogen ions, which was connected with light absorption, was not performed. Therefore, the formulas proposed by Vershubskii et al. (2004) could not be used for calculating the electric potential and the concentration gradient of hydrogen ions as a function of the radiation characteristics.

The active transport, which is caused by solar radiation, is not described in photosynthesis models. This is due to the fact that nonequilibrium-statistical nonlinear models of the active transport of ions through membranes have appeared only recently (Vershubskii et al., 2004; Melkikh and Seleznev, 2005, 2006a, 2006b, 2007a, 2007b, 2008).

The present paper deals with a model of the active transport of protons and electrons, which is caused by absorption of photons, through the thylakoid membrane in chloroplasts of plants in correlation with ATP synthesis in this membrane. The proposed model is compared in detail with previous published models. A specific feature of our model is an analytical (rather than numerical) character of the deduced relationships of proton and electron flows, as well as ATP synthesis with characteristics of radiation and its interaction with the photosynthesis system. The deduced formulas are valid at any values of the light flux in the range from zero to the direct sunlight on the Earth. In equilibrium conditions, when the temperatures of radiation and the medium coincide, the flows turn to zero in our model. In future the proposed model may become part of a general model of photosynthesis, which will explicitly take into account the absorption of light. In this model, the intensity of photosynthesis reactions will be a function of radiation characteristics, specifically, the brightness temperature.

On the other hand, despite the aforementioned models, statistical and thermodynamic analysis of photosynthesis processes is not complete either. To what extent is this process reversible? What is the efficiency of the light energy conversion process? Why is the electric potential at the membrane small, but nonzero? To answer these and other questions, we have constructed a stationary nonlinear analytical model of the light energy conversion, which was used for calculating the electric potential at the chloroplast membrane. We also analyzed ATP synthesis implemented due to the difference between the electrochemical potentials of protons.

1. A general method for calculating internal concentrations of ions and the resting potential in cells and compartments

A traditional method for calculating the resting potential was proposed in (Hodgkin and Katz, 1949). This method is oriented at experimental data on concentrations of ions outside and inside a