NUMERICAL SIMULATION OF CHLOROPHYLL A FLUORESCENCE INDUCTION IN PLANTS

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1. Introduction

Chlorophyll a fluorescence emitted by green plants reflects photosynthetic activity in a complex manner [1,2]. Illumination with continuous actinic light results in characteristic polyphasic time-course of the fluorescence yield, a phenomenon known as fluorescence induction or transient [2-4]. The fast phase of fluorescence induction, observed during the first second of illumination, has been the subject of theoretical treatment [5-9]. In this paper, we present simulation results obtained with a model centred on redox reactions of acceptor and donor sides of PSII (see Fig.1).

Fig. 1. Scheme of electron transport reactions considered in the model. CHL a: chlorophyll a antenna; OEC: oxygen evolving complex in S_n states; Y_Z: primary electron donor to $P680^+$; P680: reaction centre of PSII; Phe:pheophytin a; Q_A: primary bound plastoquinone; Q_B: secondary bound plastoquinone; PQ: plastoquinone from pool; PSI: photosystem I.
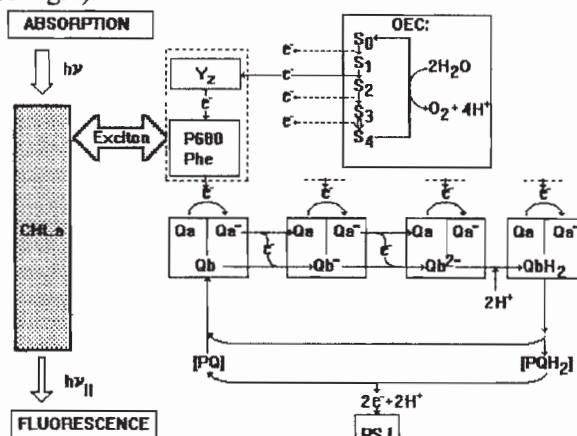
2. The model

The main assumptions of the model are: (1) Chl a variable fluorescence is related mainly to PSII kinetics [2]; (2) the net rate of Q_A reduction is higher in S_0 and S_1 than in S_2 and S_3 states of OEC [4]; (3) the relative variable fluorescence $V_t = (F_t-F_0)/(F_M-F_0)$ depends on the fraction of closed reaction centres $B(= [Q_A^-]/[Q_A]_{tot})$; the relation used is $V_t = B/(1+C(1-B))$, with $C = p_S F_V/F_0 = p_J/(1-p_J)$ (where p_S and p_J are the probabilities of connectivity between PSII units, based on the formula of Strasser (s) and Joliot (j) [10,11]); and (4) Chl a fluorescence is quenched by oxidised PQ [12]. For this type of quenching, the values of V_t were corrected by using Stern-Volmer relationship.

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The ordinary differential equations system, associated with the reactions considered in the model, was solved numerically with a specialised simulation software Gepasi [13]. The input parameters in the simulation program are the initial concentrations of reactants and the rate constants of reactions. The values of these parameters used in simulations, and the corresponding values from literature, are shown in Table 1.

Table 1. The values of input parameters used in simulations, and the corresponding values from literature (k is the rate constant of forward reaction; $t_{1/2}$ is the half time; and K_{eq} is the equilibrium constant).

Input parameters	In simulations:		From literature	
	[1]dark adapted	[2]light adapted		
Number of molecules in PQ pool	5	5	5-10	[2]
$[S_1Q_AQ_B]_i:[S_0Q_AQ_B^-]_i$	0.85:0.15	0.8:0.2	0.87:0.13 (pH=7.5)	[19]
k (or $t_{1/2}$); K_{eq} for $Q_A^-Q_B \leftrightarrow Q_AQ_B^-$	3000 s^{-1}(230 μs);50	3000 s^{-1}(230 μs);50	100-200 μs; 20	[18]
k (or $t_{1/2}$); K_{eq} for $Q_A^-Q_B^- \leftrightarrow Q_AQ_B^{2-}$	1500 s^{-1}(460 μs);10	1500 s^{-1}(460 μs); 1	300-500 μs; 1-50	[18]
k (or $t_{1/2}$); K_{eq} for $Q_B^{2-} \leftrightarrow Q_BH_2$	1300 s^{-1}(530 μs);10	1300 s^{-1}(530 μs); 1	1300 s^{-1};10 or 1	[20]
k (or $t_{1/2}$); K_{eq} for $Q_BH_2 + PQ \leftrightarrow Q_B + PQH_2$	100 s^{-1}(1.3 ms); 1	100 s^{-1}(1.3 ms); 1	*1 ms; 1	[18]
k (or $t_{1/2}$) for $PQH_2 \rightarrow PQ$	70 s^{-1}(10 ms)	200 s^{-1} (3.5 ms)	2-5 ms/e$^-$	[18]
k (or $t_{1/2}$) for $S_3 \leftrightarrow S_4 \rightarrow S_0$	700 s^{-1}(1 ms)	500 s^{-1}(1.3 ms)	1-1.3 ms 2 ms	[19] [18]

[1] leaves dark adapted 10 min before the measurement [14];
[2] leaves illuminated for 1h, and then dark adapted for 30 sec before the measurement [14];
*the half time of this second order reaction is: $t_{1/2} = \ln2/(k^*[PQ]_i)$

The rate constants of Q_A reduction are not simple. They depend, among other parameters, on: the light intensity, cross section of the antenna of PS II units, the rate constants of the primary charge separation, and of the electron transfer from Phe to Q_A. Also, the reverse reactions represent the complex process of charge recombination. The rate constant value of Q_A reduction when OEC is in S_1 state (2000 s^{-1}) has been obtained empirically from DCMU simulated curves, knowing that in experiments V_{max} value is reached in 2 ms (for I = 600 W/m^2) [14].

3. Results and discussion

Simulated results are shown in Fig.2. The curves shown in Fig. 2A are obtained from simulations with input parameters presented in Table 1 for dark adapted plants. Curves 2-5 show the changes in time of the reaction centre concentrations of complexes with Q_A
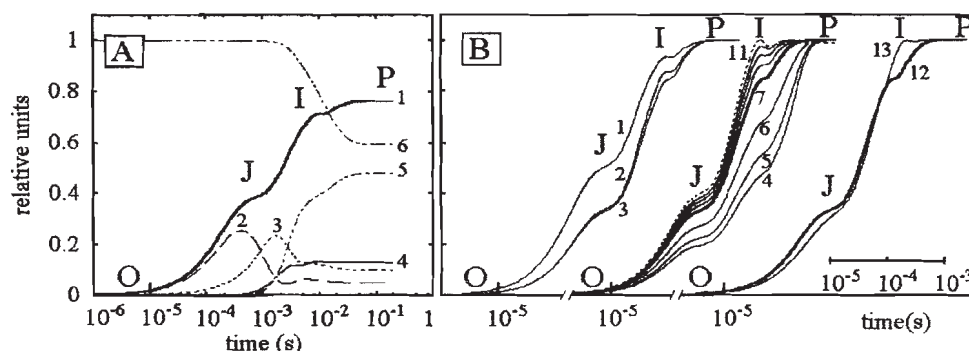
Fig. 2. A : typical curves obtained with input parameters for dark adapted condition presented in Table 1. Curves 1-6 ⇨ time variations of the concentrations of $[Q_A^-]_t$, $Q_A^-Q_B$, $Q_A^-Q_B^-$, $Q_A^-Q_B^{2-}$, $Q_A^-Q_BH_2$ and PQ/[PQ]$_{tot}$ respectively. B : Curves 1-3 ⇨ time variation of closed RCs, $[Q_A^-]_t$, the relative variable fluorescence V_t, and the relative variable fluorescence corrected for PQ quenching respectively. Curves 4-11 ⇨ time variation of the relative variable fluorescence, corrected for PQ quenching, for different values of the rate constant of oxidation of PQH_2 (0, 10, 30, 70, 100, 130, 170 and 300 s^{-1} respectively). Curves 12 and 13 ⇨ time variation of the variable fluorescence, corrected for PQ quenching, for dark adapted and light adapted values of input parameters respectively.

in its reduced form: $Q_A^-Q_B$, $Q_A^-Q_B^-$, $Q_A^-Q_B^{2-}$, and $Q_A^-Q_BH_2$ respectively. Curve 1 is the sum of these four redox forms of RCs ($[Q_A^-]_t$). We found that $Q_A^-Q_B$ is predominant at the J step. At the I and P steps all four forms of closed RCs are found in a mixture, $Q_A^-Q_BH_2$ being predominant at the P level. The PQ pool (curve 6) is reduced mostly in the I-P interval.

The effect of connectivity between PS II units, and nonphotochemical quenching by PQ, are presented in Fig.2B for dark adapted condition (curves 1, 2 and 3). The relative variable fluorescence was calculated with C = 1, corresponding to p_S = .25 and F_V/F_0 = 4 (or p_J = .5). It can be seen that PQ quenching lowers the I level.

The model presented here, in contrast to the earlier ones presented by Stirbet and Strasser [15,16], can simulate the dip after I (Fig.2B, curves 4-11), and after J (results not shown). The dip after I becomes deeper as the rate constant of plastoquinol oxidation increases (the PS I activity is enhanced). These results confirm the earlier concepts [17] that this dip is related to the dynamic equilibrium between the two photosystems. An increased number of PQ molecules in the pool also accentuates the dip (results not shown).

Curves 12 and 13 are the simulated transients obtained in dark adapted and light adapted conditions respectively. We have assumed that in light adapted condition the connectivity between PS II units is smaller (C = .25, corresponding to p_S = .125 and F_V/F_0 = 2 (or p_J = .2)). Moreover, we have used a lower value for the rate constant of Q_A reduction (1000 s^{-1} instead of 2000 s^{-1}), as the PSII absorption cross section is assumed

to be reduced. In simulated curve for light adapted condition (curve 13 in Fig.2B) V_{max} level is obtained at I level, just as in the experimental data [14].

4. Concluding Remarks

In this model of the fast phase of Chl a fluorescence induction in plants, the rate constants of the reactions from the RC level are assumed to be dependent not only on the redox state of Q_A, but also on the S_n states of OEC. The shapes of the fluorescence transients have been simulated quite well, with the characteristic steps O, J, I, and P, as well as the dips. The dip after I is partially due to the S_n states, but is also correlated with the number of PQ molecules in the pool and the equilibrium dynamics between the two photosystems, being more accentuated as the number of PQ molecules is higher, and the activity of PSI is increased. The PQ nonphotochemical quenching influences the shape of the curves, decreasing I level. The simulated curves of fluorescence induction of the light adapted plants exhibit, just as in the experimental ones, only the O, J, and I levels.

We plan to apply this model to the analysis of experiments with different light intensities, preillumination, addition of inhibitors and other stress conditions. We hope to verify and predict dynamic parameters of the photosystems in photosynthesis through this non-invasive probe of chlorophyll a fluorescence.

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