

Mathematical modelling

Mathematical modelling of natural and artificial photosynthesis

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Abstract

In natural photosynthesis solar energy is converted into chemical energy. The central part in this reaction is Photosystem II, where electrons are removed from water molecules, creating oxygen and protons. The protons are through Photosystem I used to create carbohydrates of carbon dioxide.

In artificial photosynthesis scientists try to mimic Photosystem II to split water into oxygen and hydrogen. The hydrogen can then be used as fuel.

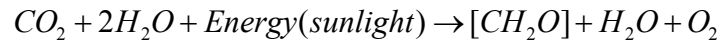
Mathematical models are here presented for the natural photosynthesis and the artificial photosynthesis.

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1. Photosynthesis in the nature

This energy harvesting reaction is one of the most important reactions on our earth. The photosynthesis let plants and cyanobacteria absorb energy from the sun and bind it chemically. That is the basis for all higher living species. Even the energy in fossil fuels, for example gasoline, is stored energy in plants, from million years ago. This reaction can be described as:



here $[CH_2O]$ is 1/6 of a sugar molecule.

This is of course just a summation and simplification of a more complicated reaction. In fact this reaction is quite complicated. It doesn't occur spontaneously, so it must be catalyzed. This is done by the organic catalyst Chlorophyll. In this project we focus on the photosynthesis in plants, called *cytosol*. The reactions takes place in a special organelle called chloroplast. The chloroplast is an ellipsoid structure enclosed in a double layer of membranes. The inner membrane form structures called thylacoids, here central parts of the photosynthetic reactions take place. We differentiate reaction cycles called Photosystem I (PS1), Photosystem II (PS2) and the Oxygen Evolving Complex (OEC).

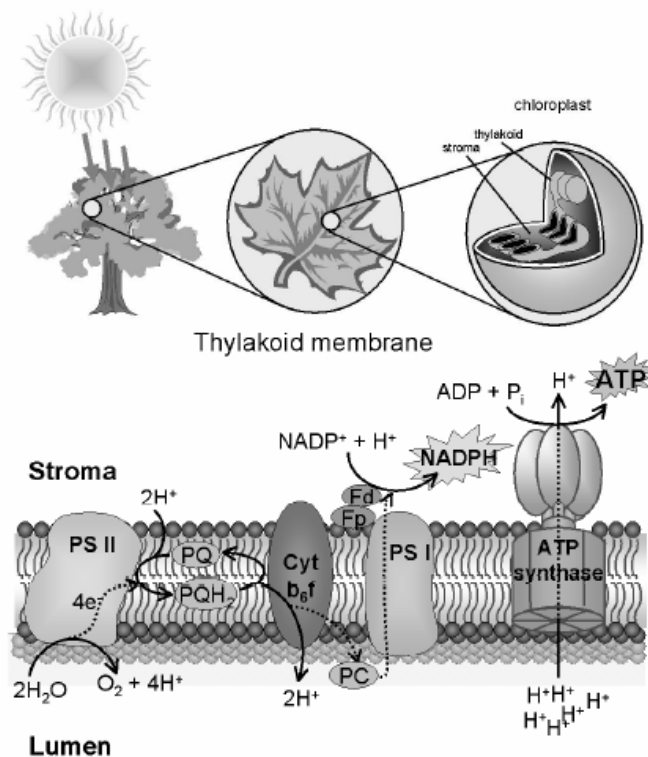


Figure 1: Schematic picture of the chloroplast and thylakoid membrane, showing the four protein complexes involved in the photosynthetic light reactions: PS II, the Cyt b6f complex, PS I and ATP synthase. The electron transfer through the system is indicated with dashed lines.

1.1 Photosystem II (PS II)

PS II is a reaction cycle including a large protein complex that consists of several protein subunits of which many constitute the light-harvesting complex. This light absorbing complex is a large antenna, consisting of several hundreds of light absorbing pigments like chlorophylls and carotenoids, whose function is to capture the solar energy and transfer it towards the place where the photosynthesis starts, i.e. the *reaction center*. When the energy reaches the reaction center it is transferred to the photoactive chlorophylls, called P680, which are excited. The excited P680* is then oxidized through an electron transfer reaction to a primary acceptor, the pheophytine (Phe), creating a charge-separated state, $P680^+ Phe^-$. The lifetime of this state is crucial for the success of photosynthesis and it is therefore important that recombination is prevented. However, to be able to absorb more solar energy and to carry out photosynthesis, the oxidized $P680^+$ needs to be reduced. $P680^+$ is then reduced through an electron transfer from a nearby tyrosine residue (Tyr), resulting in the original P680 and a neutral tyrosine radical. The electron on the Phe^- is stepwise transferred away from $P680^+$ ending up on the second quinone molecules, Qb, which increases the distance between the charges even more. The tyrosine radical oxidizes the manganese cluster (Mn_4), which has a crucial role on the electron donor side of PS II in that it is able to abstract electrons from water. The tyrosine is an intermediate reactant in the electron transfer from the manganese cluster to the oxidized $P680^+$. During the light induced charge separation cycles, the manganese cluster provides electrons for the reduction of P680 and stores up to four oxidizing equivalents. This results in the oxidation of two water molecules producing four electrons, four protons and one molecule of oxygen, and returns the manganese cluster to its most reduced state.

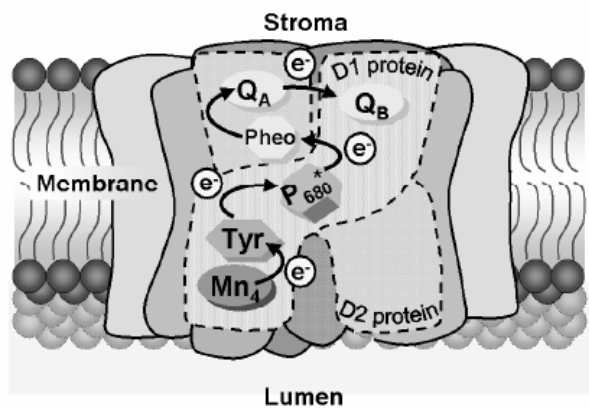


Figure 2: Schematic figure of the PS II reaction center positioned in the thylakoid membrane. The arrows indicate the light induced electron transfer reactions resulting in the oxidation of water.

1.2 The Oxygen Evolving Complex (OEC)

The manganese cluster is the catalytic center of the water splitting enzyme in natural photosynthesis. Together with the part of the PS II protein complex directly involved in the water splitting it is denoted the *oxygen-evolving complex* (OEC). The cluster consists of four manganese ions and oxygen atoms that serve as a charge accumulator. The positive charge from the photo induced charge separation process is used to extract electrons from water with the result that water is oxidized to oxygen and protons in a four-electron process.

1.3 Photosystem I (PS I)

As in PS II, antennas absorb light energy and funnel it to the reaction center of PS I resulting in excitation of a chlorophyll called P700. As in PS II the primary event at this reaction center is a light-induced separation of charge, generating a very strong reductant which leads to the production of NADPH (NADPH and ATP is energy transporters in organic life) and $P700^+$, which captures an electron from PS II to return to $P700$ so it can be excited again. When the final quinone in PS II, Qb, has received the second electron from Qa, it takes up two protons from the stroma generating QBH₂, which leaves the PS II site and is then replaced by an oxidized Qb from the membrane pool. At this point the energy of two photons has been safely and efficiently stored in the reducing potential of PQH₂. The interplay of the Qa and Qb sites enables a two-electron reduction (PQ to PQH₂) to be efficiently carried out with one-electron input. PQH₂ transfers its electrons to *plastocyanin* (PC) and PS I, a reaction catalyzed by *Cytochrome b6f* (Cyt *b6f*), and concomitantly pumps protons across the thylakoid membrane generating the proton gradient that drives the formation of ATP.

The strong reductant in the charge-separated state results in the reduction of ferredoxin (Fd), a water-soluble protein. This reaction occurs on the stromal side of the thylakoid membrane and the high potential electrons of two Fd molecules are then transferred to $NADP^+$ forming NADPH. ATP and NADPH, the products of the light reactions, are then used when CO_2 is converted into carbohydrate.

In this modelling task we have chosen to focus on the Photosystem II reaction cycle. This is a very central part for the splitting of water and scientists are now working on methods to modify the photosynthetic reactions in a way that water is split to hydrogen fuel

2. Artificial Photosynthesis

What we call artificial photosynthesis is the attempts to mimic the natural photosynthesis and split water into hydrogen with help of energy from the sun. Why is this idea so appealing? It is because, that would give an energy resource that would hold until the sun ends shining. It would also be a clean energy resource that would have very little impact on the environment.

There are several different approaches to create artificial photosynthesis, but most of the methods have lots of common components with the natural photosynthesis. Most systems have an antenna for harvesting light, a reaction center for charge separation, catalysis and a membrane to separate the generated products. The reaction is very similar to natural photosynthesis but some reactants must be changed. The P700 molecule must be modified to build hydrogen instead of building sugar.

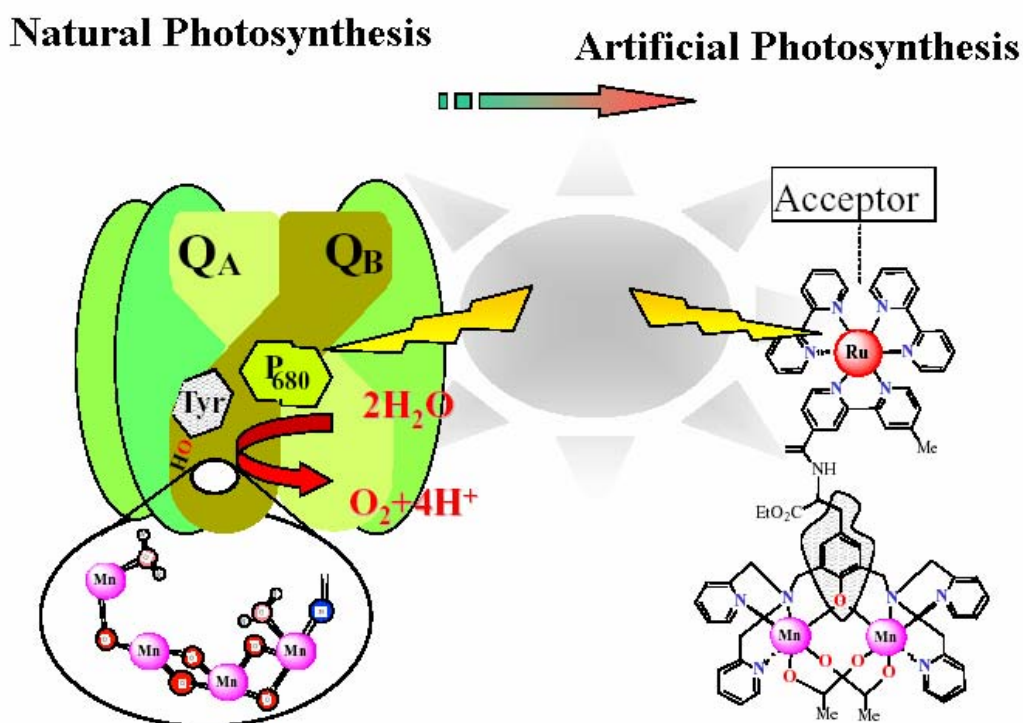


Figure 3: An illustration of the natural and artificial photosynthesis.

Key elements in the reaction are the D-A reactions (Donor, Acceptor). Scientists try with different methods to create this reaction. Most common is the method to use complexes of Ruthenium(II, III) linked to a Manganese complex as electron donor, this is done in the schematic picture, Figure 4.

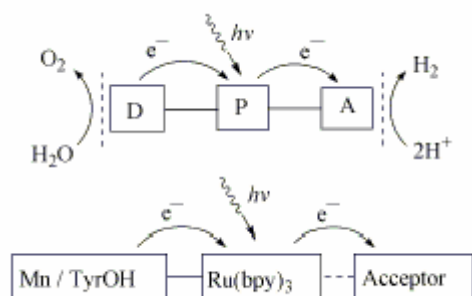


Figure 4: Schematic presentation of the electron transfer processes in an artificial photosynthetic system built on supramolecular Ru–Mn complexes.

Also Osmosium(II) or nanocrystalline TiO₂ film are used as acceptors in other methods.

In our model we use Mn-Ru(bpy)(III). Crucial for this reaction to work is that when an electron jumps away from the Ru-center, a new one must jump over from the Mn-part. Since the Mn and Ru are linked in the same molecule, a so called intramolecular reaction can occur. Those reactions are very rapid, in some experiments reaction times in nanoseconds has been measured. One of the biggest problems scientists are facing, is that a water molecule can not be split with just one electron, the Mn complex must first leave four electrons before it can react with water and split it into oxygen and hydrogen. Today scientists have managed the Ru-part to take up to three electrons. A clue may be the involving of Tyrosine. The understanding of how this part of the Mn complex catalyses the reaction, is yet a bit unknown. The problem to find an acceptor for the electrons is not yet solved, but seems not to be hard to solve.

3. Natural and Artificial Photosynthesis

A brief summary of what happens in PS II, natural photosynthesis compared with artificial photosynthesis.

Step 1: Energy from the sun is trapped by an antenna system. From here the energy is transported to the place in the molecule where the photosynthesis starts.

In natural photosynthesis this occur in (N): **Chlorophyll**
 In artificial photosynthesis this occur in (A): **Ru-complex**

Step 2: The photons are now in a photoactive pigment P. This pigment now uses the energy in the photons to give away an electron to an acceptor molecule A_1 , from were the electron keeps moving to A_2 .

N: Chlorophyll
A: Ru-complex

Step 3: For P to be able to receive more energy from the sun, an electron is transported from the amino acid Tyrosine, to P.

N: Tyrosine

A: Tyrosine z

Step 4: Tyrosine gets back the excited electron from a manganese cluster.

N: Manganese cluster

A: Manganese molecule (this part is not yet completely functional today)

Step 5: After the manganese cluster has given away four electrons, the cluster takes four electrons from two water molecules. $2H_2O \rightarrow 4H^+ + O_2 + 4e^-$.

N: Manganese cluster takes electrons from water

A: Manganese molecule takes electrons from water

Step 6: Products.

N: Carbohydrates are created through another system

A: Hydrogen molecules are created through another system
(this part is not yet functional today)

4. Modelling Natural Photosynthesis

The primary reaction of photosynthesis is located in the green-plants chloroplast, where the electron transport occurs. The mathematical approach for modelling the photosynthesis (or just PS II in our case) is to describe the electron and energy transitions. A mathematical description of the electron transfer processes and energy transition is presented in this and next chapter.

4.1 The mathematical approach

The electrons are transported in a molecular complex, and the state of the complex can be described by the electron carriers C_i , giving the state (inside the blocks) $[C_1 C_2 \dots C_n]$.

Transitions between the states can be described by ordinary differential equations:

$$\frac{dp_i}{dt} = \sum_{j=1}^l (p_j k_{ji} - p_i k_{ij})$$

Where the initial probabilities are $p_i(0) = b_i$, $i = 1, 2, \dots, l$ and k_{ij} is the constant transfer rate from i to j , or in vectorial form:

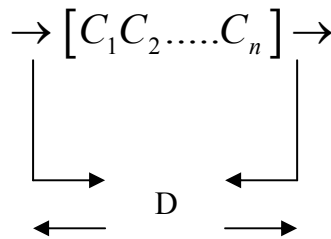
$$\frac{dP}{dt} = K^T P, P(0) = B$$

and the probability to find carrier q:

$$P_q(G) = \sum_{S_q \in G} p(S_q)$$

A photosynthetic complex contains several components, presented in either oxidized or reduced form, sometimes they can also be in excited or protonized form. The whole electron transport chain contains both PS I and PS II and is interacted by mobile carriers like plastoquinone and plastocyanin.

The electron transfer between the complex and the carriers can be described as it is in the following scheme:



and can be described by the equation:

$$\frac{d[D^-]}{dt} = k_2 [C_n^-] [D^+] - k_{-2} [D^-] [C_n^+] - k_1 [D^-] [C_1^+] + k_{-1} [C_1^-] [D^+]$$

Where $k_{\pm i}$ are rate constants, $[D^+]$, $[D^-]$ are concentrations of the mobile carrier in the oxidized and reduced forms, $[C_1^+]$, $[C_1^-]$, $[C_n^+]$ and $[C_n^-]$ are concentrations of the components of the complex, interacting with the carriers.

4.2 The model

In the model of PS2 the dynamics of the complexes can be described in terms of the dynamic probabilities of its possible states. Their interaction with the electron carriers is described according to the approach mentioned above. A detailed scheme of the process is illustrated in Figure 5.

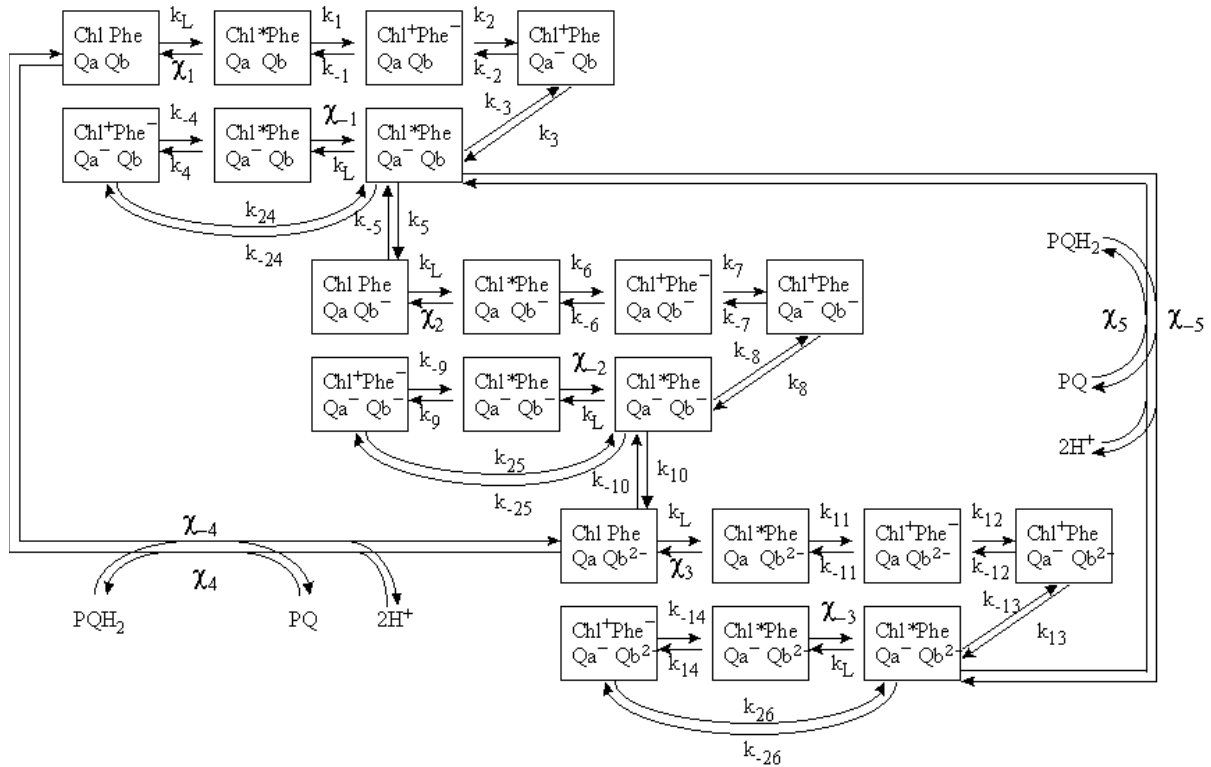


Figure 5: Detailed scheme of the photosynthetic process in PS II. Chl – chlorophyll, Phe – primary electron acceptor, Qa – primary quinone acceptor, Qb – secondary quinone acceptor, k_L - rate constant of the light reaction, $k_{\pm i}$ - rate constant of the electron transfer, $x_{\pm i}$, $i=1,2,3$ - rate constants of the deactivation from excited states, $x_{\pm 4}$ and $x_{\pm 5}$ rate constants of the electron exchange between the molecule and the electron carriers.

And a simplified scheme is illustrated in Figure 6.

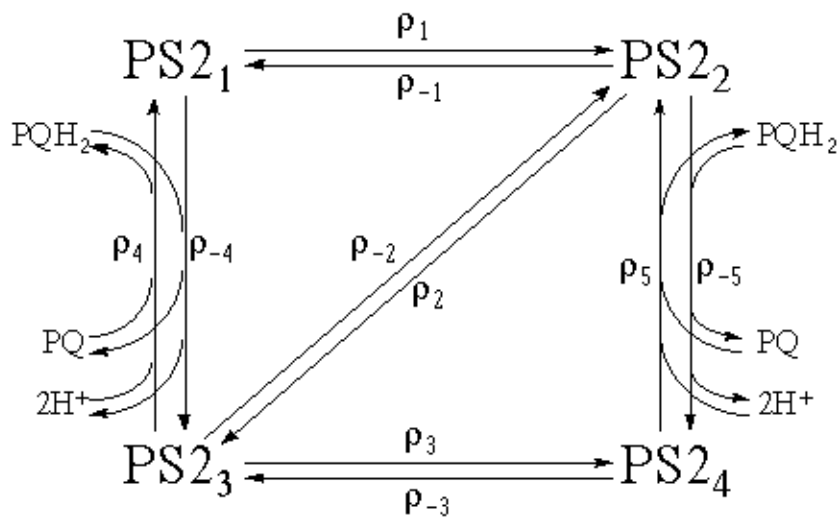


Figure 6: A simplified scheme of Figure 5.

In this simplified scheme, every state is the sum of concentrations over several states from the detailed scheme:

$$PS2_1 = \begin{bmatrix} Chl & Phe \\ Qa & Qb \end{bmatrix}$$

$$PS2_2 = \begin{bmatrix} Chl^* & Phe \\ Qa & Qb \end{bmatrix} + \begin{bmatrix} Chl^+ & Phe^- \\ Qa & Qb \end{bmatrix} + \begin{bmatrix} Chl^+ & Phe \\ Qa^- & Qb \end{bmatrix} + \begin{bmatrix} Chl & Phe \\ Qa^- & Qb \end{bmatrix} + \\ + \begin{bmatrix} Chl^* & Phe \\ Qa^- & Qb \end{bmatrix} + \begin{bmatrix} Chl^+ & Phe^- \\ Qa^- & Qb \end{bmatrix} + \begin{bmatrix} Chl & Phe \\ Qa & Qb^- \end{bmatrix}$$

$$PS2_3 = \begin{bmatrix} Chl^* & Phe \\ Qa & Qb^- \end{bmatrix} + \begin{bmatrix} Chl^+ & Phe^- \\ Qa & Qb^- \end{bmatrix} + \begin{bmatrix} Chl^+ & Phe \\ Qa^- & Qb^- \end{bmatrix} + \begin{bmatrix} Chl & Phe \\ Qa^- & Qb^- \end{bmatrix} + \\ + \begin{bmatrix} Chl^* & Phe \\ Qa^- & Qb^- \end{bmatrix} + \begin{bmatrix} Chl^+ & Phe^- \\ Qa^- & Qb^- \end{bmatrix} + \begin{bmatrix} Chl & Phe \\ Qa & Qb^{2-} \end{bmatrix}$$

$$PS2_4 = \begin{bmatrix} Chl^* & Phe \\ Qa & Qb^{2-} \end{bmatrix} + \begin{bmatrix} Chl^+ & Phe^- \\ Qa & Qb^{2-} \end{bmatrix} + \begin{bmatrix} Chl^+ & Phe \\ Qa^- & Qb^{2-} \end{bmatrix} + \begin{bmatrix} Chl & Phe \\ Qa^- & Qb^{2-} \end{bmatrix} + \\ + \begin{bmatrix} Chl^* & Phe \\ Qa^- & Qb^{2-} \end{bmatrix} + \begin{bmatrix} Chl^+ & Phe^- \\ Qa^- & Qb^{2-} \end{bmatrix}$$

The following sets of equations describe the change in concentrations in the simplified scheme:

$$PS2_1 : \dot{y}_1 = \rho_{-1} [H_p^+] y_2 + \rho_4 y_3 [PQ] [H_n^+]^2 - (\rho_1 + \rho_{-4} [PQH_2]) y_1$$

$$PS2_2 : \dot{y}_2 = \rho_1 y_1 + \rho_5 y_4 [PQ] [H_n^+]^2 + \rho_{-2} y_3 [H_p^+] - (\rho_{-1} [H_p^+] + \rho_{-5} [PQH_2] + \rho_2) y_2$$

$$PS2_3 : \dot{y}_3 = \rho_2 y_2 + \rho_{-4} y_1 [PQH_2] + \rho_{-3} [H_p^+] y_4 - (\rho_{-2} [H_p^+] + \rho_4 [PQ] [H_n^+] + \rho_3) y_3$$

$$PS2_4 : \dot{y}_4 = \rho_3 y_3 + \rho_{-5} [PQH_2] y_2 + (\rho_{-3} [H_p^+] + \rho_5 [PQ] [H_n^+]^2) y_4$$

The rate constants $\rho_{\pm i}$ are functions of the slow stages (k_{Lj} and $x_{\pm k}$ for $j = 1, \dots, 6$ and $k = 4, 5$), that are not intramolecular:

$$\rho_{-1} = \frac{x_1 / R_1}{K_1 K_2 K_3 K_5}$$

$$\rho_1 = k_{L1}$$

$$\rho_{-2} = \frac{x_2 / R_2}{K_6 K_7 K_8 K_{10}}$$

$$\rho_2 = k_{L3} / R_1$$

$$\rho_{-3} = \frac{1/R_3}{K_1 K_2 K_3} \cdot \frac{x_1 x_5 x_{-4} k_{L5}}{x_{-5} x_4 k_{L1}}$$

$$\rho_3 = k_{L5} / R_2$$

$$\rho_{-4} = x_{-4}$$

$$\rho_4 = x_4 / R_2$$

$$\rho_{-5} = \frac{x_{-5} / R_1}{K_5}$$

$$\rho_5 = x_5 / R_3$$

where $K_i = \frac{k_i}{k_{-i}}$ is the equilibrium constants for the fast stages, and:

$$R_1 = 1 + \frac{1}{K_5} + \frac{1}{K_3 K_5} + \frac{1}{K_2 K_3 K_5} + \frac{1}{K_1 K_2 K_3 K_5} + \frac{k_{L2}(1+K_4)}{x_{-1} K_5}$$

$$R_2 = 1 + \frac{1}{K_{10}} + \frac{1}{K_8 K_{10}} + \frac{1}{K_7 K_8 K_{10}} + \frac{1}{K_6 K_7 K_8 K_{10}} + \frac{k_{L4}(1+K_9)}{x_{-2} K_{10}}$$

$$R_3 = 1 + \frac{1}{K_{13}} + \frac{1}{K_{12} K_{13}} + \frac{k_{L6}(1+K_{14})}{x_{-3}} + \frac{1}{K_1 K_2 K_3} \frac{x_1 x_5 x_{-4} k_{L5}}{x_3 x_{-5} x_4 k_{L1}}$$

The intensity of the fluorescence is proportional to the excited states in PS II multiplied by their corresponding inactivation rate:

$$F = x_1 \begin{bmatrix} Chl^* & Phe \\ Qa & Qb \end{bmatrix} + x_{-1} \begin{bmatrix} Chl^* & Phe \\ Qa^- & Qb \end{bmatrix} + x_2 \begin{bmatrix} Chl^* & Phe \\ Qa & Qb^- \end{bmatrix} + x_{-2} \begin{bmatrix} Chl^* & Phe \\ Qa^- & Qb^- \end{bmatrix} +$$

$$+ x_3 \begin{bmatrix} Chl^* & Phe \\ Qa & Qb^{2-} \end{bmatrix} + x_{-3} \begin{bmatrix} Chl^* & Phe \\ Qa^- & Qb^{2-} \end{bmatrix}$$

5. Modelling Artificial Photosynthesis

Hence there is no complete system of artificial photosynthesis, our model will not either be completely accurate. We have modelled the parts of PS II that has been constructed today, and added the parts that are missing with non existing molecules. The approach is the same as for the model of the nature's photosynthesis.

5.1 The model

The difference here from the natural photosynthesis is the following:

The chlorophyll is replaced by a Ru complex (these are existing molecules), an extra electron carrier is implemented (only fictional), and after PS II the electrons are taken from water to neutralize the Ru complex, and the electrons in the fictional Qc are used to create the hydrogen molecules, this occur in another complex system. The reaction scheme will look (simplified) somewhat like Figure 7.

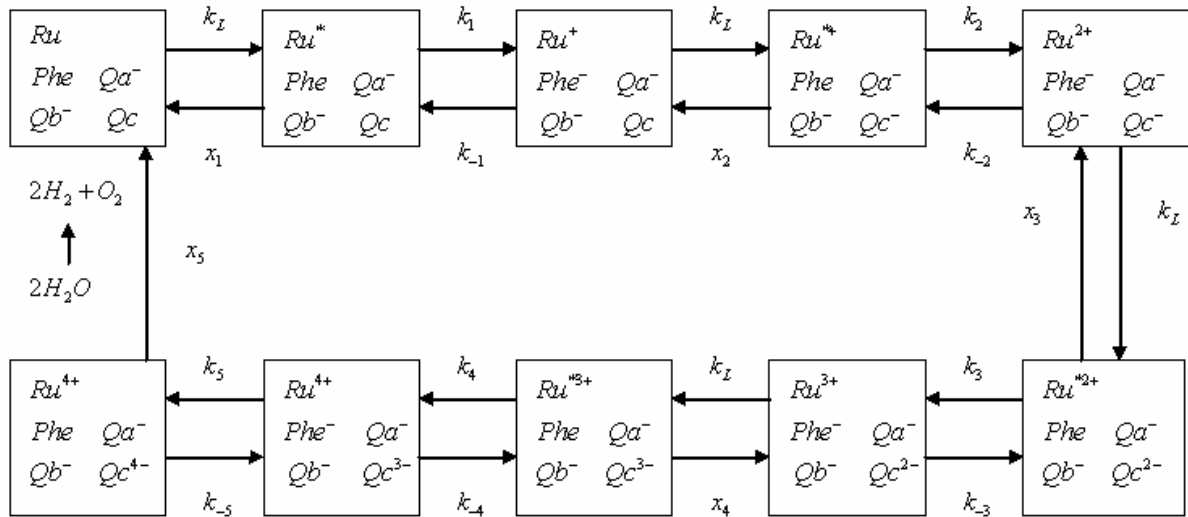


Figure 7: Detailed scheme of the artificial photosynthetic process in PS II. Ru – the Ru complex, Phe – primary electron acceptor, Qa – primary quinone acceptor, Qb – secondary quinone acceptor, Qc – imaginary quinone acceptor.

The following sets of equations describe the change in concentrations in this scheme:

$$\dot{y}_1 = x_5 \cdot y_{10} \cdot \begin{bmatrix} Ru^{4+} \\ Phe & Qa^- \\ Qb^- & Qc^{4-} \end{bmatrix} + (x_1 \cdot y_2 - y_1 \cdot k_L) \cdot \begin{bmatrix} Ru^* \\ Phe & Qa^- \\ Qb^- & Qc \end{bmatrix}$$

$$\dot{y}_2 = (k_L \cdot y_1 - x_1 \cdot y_2) \cdot \begin{bmatrix} Ru \\ Phe & Qa^- \\ Qb^- & Qc \end{bmatrix} + (k_{-1} \cdot y_3 - y_2 \cdot k_1) \cdot \begin{bmatrix} Ru^+ \\ Phe^- & Qa^- \\ Qb^- & Qc \end{bmatrix}$$

$$\begin{aligned}
\dot{y}_3 &= (k_1 \cdot y_2 - k_{-1} \cdot y_3) \cdot \begin{bmatrix} Ru^* \\ Phe & Qa^- \\ Qb^- & Qc \end{bmatrix} + (x_2 \cdot y_4 - y_3 \cdot k_L) \cdot \begin{bmatrix} Ru^{*+} \\ Phe^- & Qa^- \\ Qb^- & Qc \end{bmatrix} \\
\dot{y}_4 &= (k_L \cdot y_3 - x_2 \cdot y_4) \cdot \begin{bmatrix} Ru^+ \\ Phe^- & Qa^- \\ Qb^- & Qc \end{bmatrix} + (k_{-2} \cdot y_5 - y_4 \cdot k_2) \cdot \begin{bmatrix} Ru^{2+} \\ Phe^- & Qa^- \\ Qb^- & Qc^- \end{bmatrix} \\
\dot{y}_5 &= (k_2 \cdot y_4 - k_{-2} \cdot y_5) \cdot \begin{bmatrix} Ru^{*+} \\ Phe & Qa^- \\ Qb^- & Qc^- \end{bmatrix} + (x_3 \cdot y_6 - y_5 \cdot k_L) \cdot \begin{bmatrix} Ru^{*2+} \\ Phe & Qa^- \\ Qb^- & Qc^{2-} \end{bmatrix} \\
\dot{y}_6 &= (k_L \cdot y_5 - x_3 \cdot y_6) \cdot \begin{bmatrix} Ru^{2+} \\ Phe^- & Qa^- \\ Qb^- & Qc \end{bmatrix} + (k_{-3} \cdot y_7 - y_6 \cdot k_3) \cdot \begin{bmatrix} Ru^{3+} \\ Phe^- & Qa^- \\ Qb^- & Qc^{2-} \end{bmatrix} \\
\dot{y}_7 &= (k_3 \cdot y_6 - k_{-3} \cdot y_7) \cdot \begin{bmatrix} Ru^{*2+} \\ Phe & Qa^- \\ Qb^- & Qc^{2-} \end{bmatrix} + (x_4 \cdot y_8 - y_7 \cdot k_L) \cdot \begin{bmatrix} Ru^{*3+} \\ Phe & Qa^- \\ Qb^- & Qc^{3-} \end{bmatrix} \\
\dot{y}_8 &= (k_L \cdot y_7 - x_4 \cdot y_8) \cdot \begin{bmatrix} Ru^{3+} \\ Phe^- & Qa^- \\ Qb^- & Qc^{2-} \end{bmatrix} + (k_{-4} \cdot y_9 - y_8 \cdot k_4) \cdot \begin{bmatrix} Ru^{4+} \\ Phe & Qa^- \\ Qb^- & Qc^{4-} \end{bmatrix} \\
\dot{y}_9 &= (k_4 \cdot y_8 - k_{-4} \cdot y_9) \cdot \begin{bmatrix} Ru^{*3+} \\ Phe & Qa^- \\ Qb^- & Qc^{3-} \end{bmatrix} + (k_5 \cdot y_{10} - y_9 \cdot k_5) \cdot \begin{bmatrix} Ru^{4+} \\ Phe & Qa^- \\ Qb^- & Qc^{4-} \end{bmatrix} \\
\dot{y}_{10} &= (k_5 \cdot y_9 - k_{-5} \cdot y_{10}) \cdot \begin{bmatrix} Ru^{4+} \\ Phe^- & Qa^- \\ Qb^- & Qc^{3-} \end{bmatrix} + x_5 \cdot \begin{bmatrix} Ru \\ Phe & Qa^- \\ Qb^- & Qc \end{bmatrix}
\end{aligned}$$

The intensity of the fluorescence is proportional to the excited states in PS II multiplied by their corresponding inactivation rate:

$$F = x_1 \begin{bmatrix} Ru^* \\ Phe & Qa^- \\ Qb^- & Qc \end{bmatrix} + x_2 \begin{bmatrix} Ru^{*+} \\ Phe & Qa^- \\ Qb^- & Qc^- \end{bmatrix} + x_3 \begin{bmatrix} Ru^{*2+} \\ Phe & Qa^- \\ Qb^- & Qc^{2-} \end{bmatrix} + x_4 \begin{bmatrix} Ru^{*3+} \\ Phe & Qa^- \\ Qb^- & Qc^{3-} \end{bmatrix}$$

6. Conclusions

Mathematical models that describe Photosystem II in both natural and artificial photosynthesis have been created. Equations for the different states in the processes are defined as well as for the fluorescence. No practical measurements has been made, therefore we have no values on the reaction rates.

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