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Multiparticle Models of Brownian Dynamics for the Description of Photosynthetic Electron Transfer Involving Protein Mobile Carriers

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ABSTRACT

The article presents a review of modeling the interaction of photosynthetic proteins using the multiparticle Brownian dynamics method developed at the Department of Biophysics, Biological Faculty, Lomonosov Moscow State University. The authors used multiparticle Brownian methods coupled to molecular dynamic simulations to reveal the role of electrostatic interactions and conformational changes in the transfer of an electron from the cytochrome complex to the molecule of the mobile carrier plastocyanin in plants, green algae, and cianobacteria. Taking into account the interior of photosynthetic membrane, they developed the model, combining events of protein diffusion along the thylakoid membrane, electrostatic interactions between proteins and the proteins with the membrane charges, formation of a multiprotein complex, electron transfer within a complex, and complex dissociation. They have also developed multiparticle models of competitive interactions between electron acceptors ferredoxin.

KEYWORDS

Brownian Dynamics, Carrier, Mobile, Multiparticle Model, Photosynthetic Electron, Protein, Transfer Involving

INTRODUCTION

Photosynthetic electron transport forms the basis of light energy conversion into energy of chemical binds inside, ATP and NADPH, molecules used for metabolic needs, first of all, for CO_2 assimilation in the chloroplast of leaves and algae. Methods of mathematical and computer modeling significantly contribute to the research of the mechanisms underlying the different steps of photosynthetic electron flow to enrich the knowledge of the physical and chemical basis of energy transduction.

Traditional kinetic models, describing the electron transport chain use the apparatus of ordinary differential equations based on master equations and the mass action law (see special issue of

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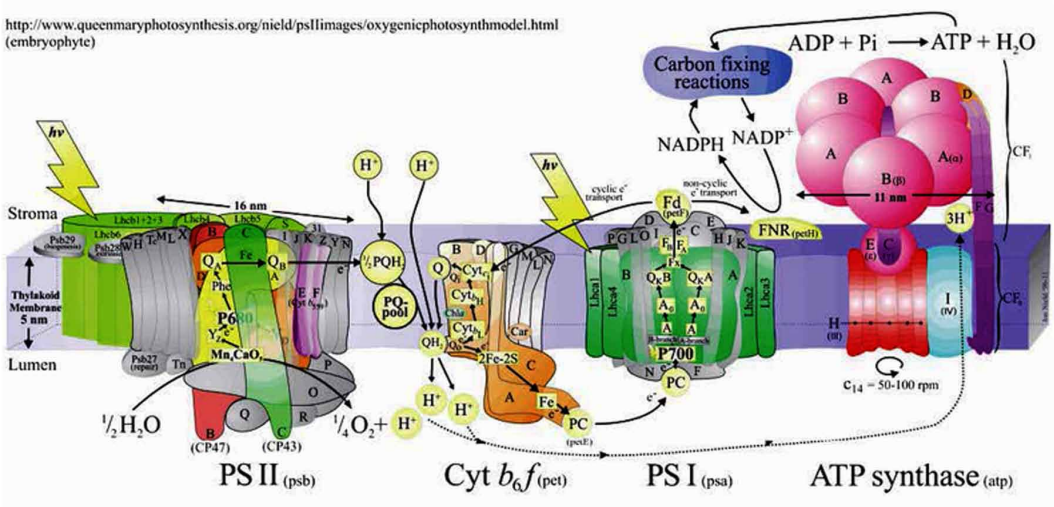
"Photosynthesis and Respiration" Series: «Photosynthesis in Silico», 2009; and (Stiurbet et al., 2014; Belyaeva et al., 2016; Rubin & Riznichenko 2014). However, the structure of the photosynthetic membrane (Figure 1) shows that in areas where electron transport is carried out by mobile carriers their interaction with multi-enzyme complexes does not comply with the concepts of free diffusion and random collisions. In a narrow luminal space, the plastocyanin (Pc) molecules, whose dimensions are comparable to the width of the luminal space, can't move freely (Haehnel et al., 1989). The same is true for the molecules of the protein ferredoxin (Fd)- mobile carrier in stromal space, which transports the electrons from PSI acceptor side to FNR and takes part in cyclic electron transfer around PSI.

To simulate the interactions of mobile electron carriers with multi-enzyme complexes in the photosynthetic membrane the method of "direct multiparticle modeling" was developed at the Department of Biophysics of the Biological Faculty together with the Department of Computer Methods in Physics of the Physics Faculty of Lomonosov Moscow State University. The main idea of this approach and the results obtained are presented in the papers (Kovalenko et al., 2006, 2010, 2011a, 2011b, 2016, 2017; Riznichenko et al., 2010; Knyazeva et al., 2010;, Ustinin et al., 2013; Khrushchev et al., 2013, 2015a, 2015b; Dyakonova et al., 2016a, 2016b; Fedorov et al., 2019) and in the book Mathematical Biophysics (Rubin & Riznichenko, 2014).

The method describes the movements of individual macromolecules - mobile electron carriers and their interaction with each other and with pigment-protein complexes embedded in photosynthetic membrane. Three-dimensional models of the protein molecules were constructed based on the data from the Protein Data Bank.

For the comparison with experimental data, such as the absorption spectrum of cell cultures, it is necessary to consider ensembles of individual macromolecules. Molecules of electron carrier proteins perform Brownian motion in a medium and electrostatically interact with each other and with the surface of a photosynthetic membrane. To simulate translational and rotational motion of molecules under the influence of random and electrostatic forces in a viscous medium the Langevin equations were used as described in (Kovalenko et al. 2006). To determine the electrostatic potential grid around each molecule Poisson–Boltzmann calculations (Ullmann & Knapp 1999) were used as described in (Knyazeva et al. 2010). For simulation of multiparticle Brownian Dynamics (BD) we have used original software ProKSim (Khruschev et al., 2013). The program is available by request; for its parameter input file also see Supporting Information (Kovalenko et al., 2017).

Figure 1. Multienzyme complexes in photosynthetic membrane. The arrows show the paths of electron transfer. (Jon Nield, http://photosynthesis.sbcs.qmul.ac.uk/nield/downloads.html)



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