Kinetic and direct computer multiparticle models of the processes in photosynthetic membrane

Galina Riznichenko, Ilja Kovalenko, Natalya Beljaeva, Alexandra Dyakonova, Anna Abaturova, Dmitry Ustinin, Andrew Rubin
Faculty of Biology, Moscow State University, 119333 Moscow GSP-2, Russia, riznich46@mail.ru

The paper presents the results of the work on kinetic and multiparticle computer modeling performed at the Dept. of Biophysics, Biological faculty MSU.

The general kinetic model of the primary photosynthetic processes in a thylakoid membrane is based on the system of ordinary differential equations, describing the processes in multi-enzyme complexes of Photosystem I, Photosystem II and Cytochrome b_6f complex, coupled to transmembrane proton and other ions transport and generation of transmembrane electrochemical potential. This model describes simultaneous kinetic changes of different variables, including concentrations of electron carriers at different redox states, electrical and electrochemical potential values; it adequately simulates a set of fluorescence induction curves experimentally recorded at different light intensities under continuous illumination and after a short laser flash.

The direct multiparticle computer models describe processes proceeding in the simulated membrane "scene", which includes stroma, lumen and intramembrane compartments constructed according to structural data. We simulate interactions of ensembles of molecules in solution and in the heterogeneous interior of a cell. In the models protein molecules move according to the laws of Brownian dynamics, mutually orient themselves in the electrical field and form complexes on the 3D scene. The method allows us to visualize the processes of molecule interactions and to evaluate the rate constants for protein complex formation reactions in the solution and in the interior of the photosynthetic membrane. 3D multiparticle computer models for simulation of complex formation kinetics for plastocyanin with photosystem 1 and cytochrome bf complex, ferredoxin with photosystem 1 and ferredoxin:$NADP^+$-reductase are considered. Effects of ionic strength are featured for wild type and mutant proteins. The computer multiparticle models demonstrate non-monotonic dependences of complex formation rates on the ionic strength as the result of long-range electrostatic interactions. The models reveal the role complex geometry of the interacting proteins and spatial organization of photosynthetic membrane.

Kinetic and multiparticle computer models allow us to evaluate the parameters of photosynthetic processes with can not be determined experimentally and reveal physical mechanism of regulation of photosynthetic electron transport and coupled processes of energy transformation.

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