Direct multiparticle models of photosynthetic protein interactions

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For understanding the regulation mechanisms on the level of whole thylakoid membrane it is useful to integrate kinetic and structural data in the computer model of the complete system. Special interest must be focused on the role of space organization of thylakoid membrane. Taking into account the heterogeneity of thylakoid membrane and the fact that the sizes of mobile carrier's molecules are comparable to the thickness of the membrane and lumen area, it becomes obvious, that chemical kinetics equations are oversimplified. In collaboration with the Dept. of Computer Methods in Physics of the Physical faculty of MSU we develop the new approach to the simulation of photosynthetic electron-transport processes. The model presents the 3D-scene, consisting of three compartments: stroma, membrane and lumen. Photosystem I (PS1), Photosystem II (PSII), cytochrome and other complexes are imbedded in membrane according to experimental data. The electron transport inside the complexes is described by differential equations for the state probabilities. Movement of mobile carriers plastoquinone molecules inside the membrane, plastocianin (Pc) molecules in lumen and ferrodoxin (Fd) molecules in stroma is described by the formalism of Brownian dynamics. The interactions between mobile proteins and embedded in the membrane multienzyme complexes includes the electrostatic interactions of the local charges of the molecules with the other molecules and the lipids of photosynthetic membrane. Direct multiparticle model gives the possibility to follow the travel of individual mobile molecule as well as to present kinetic and statistical characteristics of the system and to visualize the whole scene of the processes observed. The interactions of Pc-cytochrome f, Pc – PSI, PSI – Fd, Fd-FNR in solution and interactions of Pc-Cytf, Pc-PSI in solution and in lumen were simulated. The model was employed to assess the dependence of the association rate constant for Pc-Cytf complex formation on the dimentions of the lumen. Highest rates were obtained at the lumen span of 8-10 nm; narrowing of the lumen below 7 nm resulted in drastic deceleration of complexing. This corresponds to the experimentally observed effect of hyperosmotic stress on the interaction between Pc and Cyt f in thylakoid. Supported by RFBR grants NN 08-04-00354, 07-04-00375.