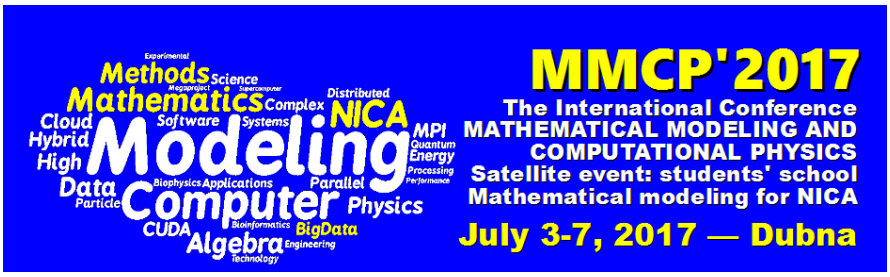

Contribution ID: **32** Type: **not specified**

Kinetic, Monte-Carlo and Multiparticle Models of the Processes in Photosynthetic Membrane

Friday 7 July 2017 08:00 (30 minutes)

Processes in photosynthetic membrane proceed at wide time scales from 10-12s-1 (charge separation in photosynthetic reaction centers of Photosystems I and II) till dozen of milliseconds (interactions with Calvin-Benson cycle of CO2 fixation).

The paper presents the results of the work on kinetic and computer modeling performed at the Dept. of Biophysics, Biological faculty MSU. Kinetic models of the primary photosynthetic processes in thylakoid membrane are based on systems of ordinary differential equations, describing the processes in multi-enzyme complexes of Photosystem I, Photosystem II and Cytochrome b6f complex, coupled to transmembrane proton and other ions transport and generation of transmembrane electrochemical potential. These models describe simultaneous kinetic changes of different variables, including concentrations of electron carriers at different redox states, electrical and electrochemical potential values; fluorescence induction and adequately simulates a set of fluorescence induction curves experimentally recorded at different light intensities under continuous illumination and after a short laser flash.

Monte-Carlo models simulate the consequence of individual elementary stages of electron-transport processes in ensembles of several millions electron transport chains, which number is comparable with the number of photosynthetic reaction centers in a real algae cell. Models of this type could be simply modified according to the data of electron transport chain organization at different growth conditions.

The multiparticle computer models describe processes proceeding in the simulated membrane "scene", which includes stroma, lumen and in transmembrane 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. After the interacting molecules approach each other and produce the preliminary complex, we switch off molecular dynamic procedure to simulate intermolecular conformation activity leading to the formation of the final complex, in which the redox reaction occurs. The method allows 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 of interactions Cytf-Pc and Pc-PSI in lumen of thylakoid, taking into account the influence of the charge of the membrane, are developed. Directed electron transport Cytf–PSI via Pc is simulated according to experimental data. The models reveal the role of complex geometry of the interacting proteins and spatial organization of photosynthetic membrane.

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

The work was supported by grants of the RFBR (grants N 14-04-00302, 14-04-00326, 17-04-00676)

Short biography note

Professor of Lomonosov Moscow State University

Author: Prof. RIZNICHENKO, Galina (Lomonosov Moscow State University, MSU)

Presenter: Prof. RIZNICHENKO, Galina (Lomonosov Moscow State University, MSU)

Session Classification: Plenary