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Use of a system of differential equations to analyze the functioning of a catalytic biomacromolecule under nonequilibrium conditions.

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Structural-dynamic properties of biomacromolecules in nonequilibrium conditions of functioning determine the kinetics of their main reaction on external action. Such kinetics is a multi-exponential. This is due both to the possible functioning of various subsystems in the macromolecules structure, and to the influence of main reaction on the macromolecules structure.

This can be explained by action of the macromolecule stationary states, which are represented as mono exponential components of the main reaction.

The most interesting case is when the parameters of such components depend not only on the parameters of external action, but can be correlated among themselves. In this case using just exponential components it is not possible to reliably identify the subsystems of macromolecule. Using the parameters of exponential components, further detailing of the main reaction was carried out by building a system of differential equations.The algorithm and calculation program are developed on the basis of experimental kinetics analysis of cyclic photostimulated electron transfer in isolated reaction centers (RC) Rhodobacter sphaeroides. The data of this kinetics was used for building an optimization process of the inverse problem solving. For this purpose the measured kinetics of cyclic electron transfer was approximated by a sum of three exponential functions [1] separately for the processes of RC photoexcitation and RC relaxation. Using the values of exponential functions parameters as a solution for differential equations system, the inverse problem was solved by obtaining the coefficients for three differential equations system and the equation of state. Knowing the constant coefficients values of differential equations system the occupancy kinetics of four electronic-conformational RC substates was determined. The extremums obtained for the occupancy of RC substates are ranged from 3 to 140 ms. This can be caused by structural self-regulation effects of the main reaction as a result of macromolecules RC space-time motions.

1. *Yu. M.Barabash, A.K.Lyamets*, A Method for Decomposition of the Basic Reaction of Biological Macromolecules into Exponential Components, Nanoscale Research Letters (2016) 11:544 DOI 10.1186/s11671-016-1758-1