The method to analyze the functioning of the catalytic biomacromolecules under nonequilibrium conditions

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The aim of the work was to analyze the response of an object to an external influence by identification hidden parameters of the objects under study based on differential equations with constant coefficients.

It is known that the solution of a differential equations system with constant coefficients is expressed as a certain sum of exponential functions. If the experimental kinetics of the main reaction is described as the sum of exponential functions, then it can correspond to a certain system of differential equations. Such differential equations describe independent subsystems of the object.

As an object the reaction centers (RC) of the purple bacteria were used. The experimental kinetics of cyclic electron transfer in RC was approximated by the sum of three exponential functions with a material balance equation. They determined the number of differential equations. The parameters of the exponential functions were used to determine the values of the coefficients of the three differential equations, which were equal to the algebraic sum of the reaction rate constants for the balance equations RC. The values rate constants of the balance equations rate constants were found by solving the optimization problem using the coordinate descent method. The solution of the differential equations system determined the kinetics of RC substations populations. It allows us to determine the number of balance equations, the number and behavior kinetics of sub states (subsystems) of an object.

The task was to create a computer program (Delphi7) to identify four differential equations with constant coefficients with material equation for balance. The algorithm developed using the electron transfer kinetics of the reaction center. Another task was to determine the kinetics of electron transfer between the hidden states of the reaction center. These results are in a good agreement with the results of the reaction center study using the two exposures method.