ANALYSIS OF REACTION PHASE TRAJECTORIES FOR ESTABLISHING FUNDAMENTAL ASPECTS OF CATALYTIC SYSTEMS OPERATION

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The establishing of fundamental patterns of operation of catalytic systems of complex reactions is non-trivial scientific task because of proceeding of several coupled consecutive-parallel processes in such systems. The studies of kinetic regularities of reactions proceeding is one of the most effective tools for establishing of their mechanisms. We proposed and tested the approach based on the analysis of differential selectivity of a catalytic reaction under competition of several (pair, as minimum) similar substrates using so-called phase trajectories of the competing reactions being interdependences of the yields of the products formed in the competing reaction. [1]. The analysis of patterns of phase trajectories' changes with varying different reaction parameters, such as the nature and concentration of the substrates and components of the catalytic systems used, allows for solving a lot of questions appearing under establishing the catalytic reaction mechanism (i.e., nature of intermediates participating in the elementary steps of catalytic cycles, the degree of reversibility of the steps, a mechanism of their coupling with each other, distinguishing between homogeneous and heterogeneous catalysis mechanisms, etc.). The main advantage of the approach over traditional kinetic studies of the rates of reactions is the independence of its results on substantially changing during the reaction concentration of catalytically active species that usually cannot be measured correctly. The results of the application of the approach to several cross-coupling reactions with aryl bromides and unreactive aryl chlorides complicated by intensive processes of catalyst deactivation are discussed in the report.

References
1. Schmidt A.F., Kurokhtina A.A., Larina E.V. Catal. Sci. Technol., 2014, 4, 3439.

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