COMPLEXITY IN A KINETIC MODEL OF HETEROGENEOUS CATALYTIC REACTION WITH AN HIERARCHY OF CHARACTERISTIC TIMES.

GENNADII CHUMAKOV AND NATALIYA CHUMAKOVA

Abstract. Under study is a system of three nonlinear ordinary differential equations with fast, intermediate, and slow variables that models the dynamics of the heterogeneous catalytic reaction of hydrogen oxidation. The system accounts for the influence of the catalyst surface state on the properties and, in particular, on the activity of the catalyst. We shown this model to have a wide spectrum of the complexity phenomena.

We present some results of studying different types of the multi-peak oscillations and the chaotic behavior in the dynamical system with a hierarchy of characteristic times and illustrate that the influence of adsorbed species on the rate of catalytic reaction may lead to multi-peak oscillations and even to chaotic behavior under isothermal conditions. Such a situation occurs, for example, when the surface heterogeneity of the catalytic sites causes the activation energy of some reaction stage (or stages) to change with the surface coverage by one of the intermediate substances. Numerical simulations are used to demonstrate different types of the multipeak oscillations and chaos in the kinetic model of hydrogen oxidation on nickel catalyst.

Under study is also the behavior of the global error of numerical integration in the two-variable mathematical model of a heterogeneous catalytic reaction [1]. Numerical estimation of the global error indicates that there is a high sensitive dependence of the solutions on initial conditions due to the existence of a tunnel-type bundle of trajectories which is formed by the stable and unstable canards. We show that the exponential growth of the norm of the fundamental matrix of solutions of the system linearized around a stable canard-cycle yields exponential growth of the leading term in the global error of numerical solution

Moreover, we provide some numerical analysis of the chaotic behavior within an attractor in terms of a Poincare map. For this purpose, we study a bifurcation of an invariant torus since it is of great interest to clarify the scenario of transition from periodic behavior corresponding to a stable cycle on the torus to the regime of chaotic multi-peak oscillations [2]. Note that, before the break-down of the invariant torus for some value of the control parameter (i.e., the bifurcation of the invariant torus occurs), the torus should lose its smoothness.

Finally in this paper, we study a scheme that allows us to generate homoclinic chaos in the three-dimensional system. In this case, for the generation of chaotic dynamics we use the Feigenbaum period-doubling scenario.

References

[1] Chumakov G.A., Lashina E.A., Chumakova N.A. “On estimation of the global error of numerical solutioin on canard-cycles.”, *Mathematics and Computers in Simulation*, Vol. 116, 59-74 (2015).

[2] Chumakov G.A., Lashina E.A., Chumakova N.A. “Modeling the complex dynamics of heterogeneous catalytic reactions with fast, intermediate, and slow variables .”, *Chem. Eng. J.*, Vol. 282, 11-19 (2015).

Gennadii Aleksandrovich Chumakov
Sobolev Institute of Mathematics,
4 Acad. Koptyug avenue,
630090, Novosibirsk, Russia

Novosibirsk State University,
2 Pirogov street,
630090, Novosibirsk, Russia
E-mail address: chumakov@math.nsc.ru

Nataliya Alekseevna Chumakova
Boreskov Institute of Catalysis,
5 Acad. Lavrent'ev avenue,
630090, Novosibirsk, Russia

Novosibirsk State University,
2 Pirogov street,
630090, Novosibirsk, Russia
E-mail address: chum@catalysis.ru