

# Binary correspondences and an algorithm for solving an inverse problem of chemical kinetics in a nondegenerate case

*Gutman A. E., Kononenko L. I.*

Sobolev Institute of Mathematics, Novosibirsk State University

We consider a singularly perturbed system of ordinary differential equations which describes a process in chemical kinetics [1, 2]:

$$\begin{aligned}\dot{x}(t) &= f(x(t), y(t), t, \varepsilon), \\ \varepsilon \dot{y}(t) &= g(x(t), y(t), t, \varepsilon),\end{aligned}$$

where  $x \in \mathbb{R}^m$ ,  $y \in \mathbb{R}^n$ ,  $t \in \mathbb{R}$ ,  $\varepsilon$  is a small parameter,  $f, g$  are sufficiently smooth functions. Direct and inverse problems are stated for such a system for the case in which the right-hand sides are polynomials of arbitrary degree.

Binary correspondences are used for formalization of problems, their basic components, properties, and constructions [3, 4, 5]. It is shown how the inverse problem of chemical kinetics can be corrected and made more practical by means of the composition with a simple auxiliary problem which represents the relation between functions and finite sets of numerical parameters being measured. Formulas for the solution of the inverse problem are presented for the degenerate case  $\varepsilon = 0$  and conditions of unique solvability are indicated for the corrected inverse problem.

An iteration algorithm is proposed for finding an approximate solution to the inverse problem for the nondegenerate case  $\varepsilon \neq 0$ . At each step of the algorithm, the solution of the inverse problem for the above-considered case  $\varepsilon = 0$  is combined with the solution of the direct problem which is reduced to the proof of the existence and uniqueness of a solution in the case  $\varepsilon \neq 0$ . The conjecture is stated on convergence of the algorithm and an approach to its justification is developed which is based on the Banach fixed-point theorem.

The work was carried out in the framework of the State Task to the Sobolev Institute of Mathematics (Projects 0314–2019–0005 and 0314–2019–0007) and supported by the Russian Foundation for Basic Research (Project 18-01-00057).

## References

- [1] Vasil'eva A. V., Butuzov V. F. *Singularly perturbed equations in critical cases*. Moscow: Moscow Gos. Univ., 1978. (in Russian).
- [2] Goldstein V. M., Sobolev V. A. *Qualitative analysis of singularly perturbed systems*. Novosibirsk: Sobolev Institute of Mathematics, 1988. (in Russian).
- [3] Gutman A. E., Kononenko L. I. Formalization of inverse problems and its applications // *Sib. J. Pure. Appl. Math.* 2017. V. 17, N 4. P. 49–56. (in Russian).
- [4] Gutman A. E., Kononenko L. I. The inverse problem of chemical kinetics as a composition of binary correspondences // *Sib. Electron. Math. Rep.* 2018. V. 15. P. 48–53. (in Russian).
- [5] Gutman A. E., Kononenko L. I. Binary correspondences and the inverse problem of chemical kinetics // *Vladikavkaz Math. J.* 2018. V. 20, issue 3. P. 37–47.