



Thematic section: Theoretical Research.

Short Communication

Subsection: Physical Organic Chemistry.

The Reference Object Identifier – ROI-jbc-A/21-1-2-3

The Digital Object Identifier – DOI: 10.37952/ROI-jbc-A/21-1-2-3

Received 10 March 2021; Accepted 13 March 2021

Application of conservation laws to identify the mechanisms of chemical reactions

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Keywords: conservation laws, chemical kinetics, reaction mechanism.

Abstract

Conservation laws for chemical reactions are autonomous time-independent combinations of non-stationary concentrations of reagents and reaction parameters. They can be divided into stoichiometric and kinetic conservation laws. Stoichiometric conservation laws depend only on the stoichiometry of the reaction, reagent concentrations and initial conditions. Such conservation laws are quite simple to find and are valid for any form of the kinetic law of stages. In closed systems, the number of independent stoichiometric conservation laws is determined by the number of different atoms of the substances participating in the reaction and is equal to $N_s = n - R \geq 1$, where n is the total number of reagents; R is the rank of the matrix of stoichiometric coefficients. In open systems the number of conservation laws can be any or they can be completely absent. This article discusses conservation laws for chemical reactions proceeding unsteady in a tubular reactor with uniform diffusion of reagents in the longitudinal and radial directions. It is shown that the conservation laws for such reactions depend on the stoichiometric coefficients of the elementary stages of the mechanism, the initial and current concentrations of the reagents. At the same time various detailed mechanisms of the same reaction are characterized by different independent conservation laws, which makes it possible to use these laws to identify the mechanisms of chemical reactions. It is shown that the conservation laws make it possible to identify the mechanisms of nonlinear reactions under any kinetic laws and any number of stages. Using conservation laws, an example of choosing the most probable mechanism from several alternative reaction mechanisms is considered.

For citation: Nikolay I. Koltsov. Application of conservation laws to identify the mechanisms of chemical reactions. *Butlerov Communications A*. 2021. Vol.1. No.2. Id.3. DOI: 10.37952/ROI-jbc-A/21-1-2-3

References

- [1] B.V. Volter, I.E. Salnikov. Stability of operating modes of chemical reactors. *Moscow: Chemistry*. **1981**. 198p. (Russian)
- [2] G.S. Yablonsky, V.I. Bykov, A.N. Gorban. Kinetic models of catalytic reactions. *Novosibirsk: Science*. **1983**. 254p. (Russian)
- [3] D.A. Frank-Kamenetskiy. Basics of Macrokinetics. Diffusion and heat transfer in chemical kinetics. *Moscow: Intellect*. **2008**. 408p. (Russian)
- [4] V.I. Bykov, S.B. Tsybenova. Nonlinear models of chemical kinetics. *Moscow: URSS*. **2011**. 400p. (Russian)
- [5] M.D. Korzukhin. Linear conservation laws in chemical kinetics. *Journal of Physical Chemistry*. **1972**. Vol.46. No.7. P.1845-1847. (Russian)
- [6] N.I. Kol'tsov, B.V. Alekseev, V.Kh. Fedotov. On nonlinear conservation laws in catalytic reactions. *Journal of Physical Chemistry*. **1988**. Vol.62. No.11. P.3069-3072. (Russian)
- [7] B.V. Alekseev, N.I. Kol'tsov, V.Kh. Fedotov. Linear invariants in the formal kinetics of chemical reactions. *Journal of Physical Chemistry*. **1992**. Vol.66. No.12. P.3219-3234. (Russian)
- [8] N.I. Kol'tsov. Quasi-Invariants of Chemical Reactions in the Ideal Displacement Reactor. *Theor. Found. of Chem. Eng.* **2020**. Vol.54. No.5. P.913-918. <https://doi.org/10.1134/S004057952004020X>
- [9] N.I. Kol'tsov. Quasi-invariants of chemical reactions in distributed systems with diffusion. *Proceedings of Higher Educational Institutions. Chemistry Series Technology*. **2021**. Vol.64. No.1. P.41-46. <https://doi.org/10.6060/ivkkt.20216401.6133>
- [10] Nikolay I. Koltsov. Application of conservation laws to identify the mechanisms of chemical reactions. *Butlerov Communications*. **2021**. Vol.65. No.3. P.119-122. DOI: 10.37952/ROI-jbc-01/21-65-3-119 (Russian)