

Limit Cycles in a Two-Species Reaction*

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Abstract Kinetic differential equations, being nonlinear, are capable of producing many kinds of exotic phenomena. However, the existence of multistationarity, oscillation or chaos is usually proved by numerical methods. Here we investigate a relatively simple reaction among two species consisting of five reaction steps, one of the third order. Using symbolic methods we find the necessary and sufficient conditions on the parameters of the kinetic differential equation of the reaction under which a limit cycle bifurcates from the stationary point in the positive quadrant in a supercritical Hopf bifurcation. We also performed the search for partial integrals of the system and have found one such integral. Application of the methods needs computer help (Wolfram language and the SINGULAR computer algebra system) because the symbolic calculations to carry out are too complicated to do by hand.

Keywords Limit cycles, two-species reaction, third order reaction step.

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1. Introduction

After an extremely short review of the history of oscillatory reactions we describe how and why we selected—both from the mathematical and chemical points of view—the model investigated here. Definitions of concepts and formulation of theorems not given here can be found e.g. in [44] and [34].

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1.1. Historical remarks

Chemical reactions show all kinds of exotic behavior: oscillation, multistability, multistationarity, or chaos. They are interesting not only from the mathematical point of view, but oscillatory behavior in a reaction may also form the basis of periodic behavior in biological systems that can have different periods: minutes, one day, one year etc., see [14, 30, 31, 47]. Analogous expectations can be expressed in connection with other phenomena. Here we are only concerned with oscillatory behavior.

In his famous 1900 lecture David Hilbert formulated as the second part of his XVIth problem to find the number of limit cycles of two-dimensional autonomous polynomial differential systems, see e.g. [28]. The last more than 100 years have shown that this is a very hard problem (see e.g. [28].) However, from the point of view of applications one would need even more: find the number of periodic solutions of polynomial differential equations in any number of variables although one would be content with the solution of the kinetic case, i.e. a subclass of quadratic or cubic polynomials is only relevant. Early attacks by [17, 18] are worth mentioning here.

As it can be seen from history, Hilbert's XVIth problem seems to be very difficult even in the case of two-dimensional kinetic differential equations. (It is quite characteristic that according to Schlomiuk and Vulpe [36] in the class of quadratic differential equations—slightly larger than the set of kinetic differential equations—the number of different phase portraits is estimated to be more than two thousand.) We neglected quite important topics: the case of simplest oscillators, see e.g. [41, 43, 46], reactions with more than two species [1, 21, 42], etc.

1.1.1. Existence of periodic trajectories

Especially when the experiments of Belousov [7] became widely known—first, through the work by Zhabotinsky [48]—the question emerged what are the structural conditions of the existence of periodic solutions in a kinetic differential equation. (On the difference between structural and parametric conditions see e.g. [5, 6].)

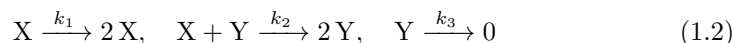
A fruitful tool to prove the existence of periodic solutions is the theorem on Andronov–Hopf bifurcation as it has been shown by Hsü [27]: he has rigorously shown that the Oregonator model of the Belousov–Zhabotinsky reaction has periodic solutions. Another early application is shown in [39] containing a reaction similar to the Brusselator—see below: (1.10)—to model synaptic low waves and having periodic solutions as a consequence of the above mentioned theorem.

Another method to prove the existence of closed trajectories is to find first integrals having closed level curves. This is how one can investigate the Lotka–Volterra reaction.

Even before oscillatory chemical reactions became popular in the seventies of the XXth century, following the work by Belousov and Zhabotinsky, and later by Field, Kőrös and Noyes [22] and others, the biologically motivated differential equation

$$\dot{x} = k_1x - k_2xy, \quad \dot{y} = k_2xy - k_3y \quad (1.1)$$

was reinterpreted as the induced kinetic differential equation of the reaction



and was used as a model of oscillation in cold flames by Frank-Kamenetsky [23].