# Computing realizations of reaction kinetic networks with given properties

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**The realization problem in reaction kinetics** Reaction kinetic systems form a special class of positive systems with smooth nonlinearities where advantageous dynamic properties, such as global may be ensured thanks to the special structure of the system model. In the classical case, these systems are described by a set of ordinary differential equations (ODEs) with polynomial right-hand sides [2, 4]. Beside the description of classical chemical reactions, reaction kinetic systems are the main building blocks of highly interconnected biochemical systems with complex behavior such as metabolic or cell signalling pathways [8].

The so-called inverse problem of reaction kinetics (i.e. the characterization of those polynomial differential equations which are kinetic) was solved in [5]. It is known from the "fundamental dogma of chemical kinetics" that different reaction networks can produce the same kinetic differential equations [6]. Naturally, this property has a fundamental impact on the identifiability of reaction rate constants [1].

However, the task of finding realization(s) with given prescribed properties, e.g. realizations with minimal number of reactions or with a given deficiency, has not attracted a lot of attention. This task will be called the *realization problem* and it is the subject of our paper.

**Realization problems in the MINLP framework** Recent studies indicate [7] that it is possible and quite useful to formulate and solve realization problems of different kinds in the framework of mixed integer linear programming (MILP) [3], where the continuous optimization variables are the nonnegative reaction rate coefficients, and the corresponding integer variables ensure the finding of the realization with the minimal or maximal number of reactions. The mass-action kinetics is expressed in the form of linear constraints adjoining the optimization problem.

However, the underlying MILP problem is NP-hard even in the above mentioned simplest realization case. More complex realization problems will require to solve mixed integer nonlinear programming problems where these computational complexity problems can be even more

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severe. Here the combinatorial structure of the problem can be utilized to develop more efficient algorithms.

**Realizations with special prescribed properties** From the viewpoint of the applications, the existence of realization(s) with given structural properties are of importance. Such structural properties include realizations with reversible reactions, with minimal number of complexes, with a given deficiency etc. From the theoretical viewpoint, the existence of a realization with a given property and the relationships between realizations possessing different structural properties is of interest.

Therefore, the following special cases are investigated:

- the existence and uniqueness of realizations with reversible reactions,
- construction of realizations with minimal number of complexes,
- the existence and uniqueness of realizations with deficiency zero and higher.

The developed results are illustrated through interesting computational examples.

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