Final report

Gábor Szederkényi, Péter Polcz, and Gergő Szlobodnyik and their colleagues have proved statements mainly using the concepts and tools of **control theory** such as reachability (Szlobodnyik et al., 2019; Szlobodnyik and Szederkényi, 2019). Concepts and methods of this theory (such as controllability, reachability) have been used to solve problems of reaction kinetics by Drexler, Virágh, and Tóth (2018).

Gábor Szederkényi, Péter Polcz and their coworkers also contributed to the **qualitative theory of differential equations** with the development of several concepts (an appropriate Lyapunov or storage function can prove stability, passivity, finite L2-gain property, or other specific dynamic behavior for general nonlinear uncertain systems, however, the algorithmic construction of such functions has not yet been solved). Polcz and Szederkényi have proved statements and developed numerical and computer algebra approaches, which allow computational stability-, domain of attraction-, passivity-, and induced L2 performance-analysis for a large class of nonlinear (rational, uncertain) dynamical models: Polcz et al. (2018, Improved...), Polcz et al. (2018, Reduced...), Polcz et al. (2019, Computational...), Polcz, Szederkényi (2021), Polcz et al. (2018, Observer-based...), Polcz et al. (2019, Passivity analysis...).

The series of papers with Dániel András Drexler as one of the authors usually concentrate on **tumor growth control** with the more realistic positive input: Drexler, Sápi, and Kovács (2018), Drexler, Nagy, Romanovsky, Tóth, and Kovács (2018), Drexler, Ferenci, Lovrics, and Kovács (2019), Drexler and Kovács (2020,2021), Puskás and Drexler (2021).

János Tóth and Ilona Nagy together with other participants of the project and also with our Slovenian coworkers have found results on the qualitative behavior (mainly: existence or non-existence of one or morelimit cycles) for **individual, parametrized models**: Nagy, Romanovski, and Tóth (2020), Fercec et al. (2019).

An important **inverse problem** of reaction kinetics is to find reactions inducing a given kinetic differential equation. The paper by Craciun et al. (2020) is a relevant contribution to the topics. Another inverse problem–model selection–is the topics of papers by Tóth, Nagy, and Ladics (2019) and Nagy, Ladics, and Tóth (2020) on automatic model selection which gives a method to help the chemist by providing all the possible models of a given set of measurements. Shavarani et al. (2020) on the positivity of concentrations also belongs to this area. Gustavo et al. (2020) applies classical methods to solve the most typical inverse problem, that of parameter estimation for enzymatic resolution in supercritical carbon dioxide. That topics is recurring in papers by the Dániel Drexler group classified elsewhere. Vághy and Szederkényi (2021) have found realizations of uncertain kinetic systems with time delay.

Formal reaction kinetics (or chemical reaction network theory) is a well developed mathematical theory of chemical reactions. However, it is worth **returning to chemical** reaction kinetics from time to time in order to avoid being not too self-contained, rather extend the mathematical methods to further areas. This is the goal of the one by Gáspár and Tóth (2021) presenting a novel general definition of reaction extent.

Some of the papers may be considered as **case studies**, e.g., or the one by Szalisznyó et al. (2019) on the dynamics in schizo-obsessive spectrum disorders, or Dukaric et al. (2018) on repressilators. Not a stand-alone paper but a starting point of further investigations is the paper by Rebeka Szabó and Lente

(2021) who have formulated and studied a **stochastic** nucleation-growth model nanoparticle formation. Another paper on the application of a stochastic model within an absolutely timely area, epidemiology, is Polcz, P. et al. (2022) in press.

Pure methodical (or: more mathematical) papers follow. Drexler, Virágh, and Tóth (2018) treated controllability and reachability of reactions. Gustavo and Tóth (2019) compared the number-crunching abilities of Matlab and Mathematica to conclude that they are similar, but obviously, Mathematica (Wolfram language) on the one hand can perform tasks unimaginable by Matlab-users, and, what is more, offers a significant reduction of human work in the average being more concise and problem-oriented. One might mention here that the present grant could also support the preparation of the third edition of a textbook on differential equations (Tóth and Simon, 2020) and writing of an English textbook (Tóth et al. 2018) on **formal reaction kinetics** summarizing recent results in the topics, presenting exercises with solutions and offering open problems for the researchers. (The earlier book by Érdi and Tóth, 1989, also contained open problems some of which have been solved by several authors.) These last two items together with Tóth (2021) aim at helping the newcomers in the field, students or reseachers, as well.

Also, 9–10 January we organized the 3rd **Workshop on Formal Reaction Kinetics and Related Problems**. The 4th Workshop had to be relegated because of the pandemic.

As far as it was possible we went on with the seminar on Formal Reaction Kinetics and Related Problems in online, offline, or hybrid form with more and more foreign participants in the seminars and in our workshops. Michael Gustavo has written his MSc thesis, and three of the participants (Gergő Szlobodnyik, Péter Polcz, and Ilona Nagy) finished their Ph.D. thesis during this period.

The participants altogether had around 60 talks at different conferences, 90 percentages in English.

To appreciate our results the following facts should be taken into consideration: we have been essentially deprived of one of our main tools, the Wolfram Language, that we used continuously in the last 30 years. Furthermore, **public procurement** usually means a 20–50% percent increase in prices compared to the prices on the market, months or even a year of delay in supply, and the impossibility to choose the specified version of tools or service. Waste of energy, time and money.

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Algebraic methods for the application of differential equations

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