

Lectures on formal reaction kinetics
and related questions 2.
9th Feb., 2018, BUTE Building H, Room no. 306

8:45– 9:00 Registration, opening gala

9:00–10:00 **Georg Regensburger** and **Stefan Müller** (Universität Wien): Generalized mass-action systems and the bijectivity of exponential maps

10:00–10:20 **Drexler András Dániel** (Óbudai Egyetem): Control of dynamical systems with positive input

There are many dynamical systems in practice whose input can only be positive, however most control algorithms can not guarantee positive input, and controllability analysis is also developed for systems whose input can have any sign. A dynamic extension of the system is given, where the original input is considered as a new state of the system whose differential equation defines a nonnegative system with a new fictitious input, and controllability analysis and control synthesis is done for the extended system. This way, positivity of the original system's input is guaranteed. The properties of a specific dynamical extension are examined and applications are shown from physiological control.

10:20–10:50 Coffee break, tea included

10:50–11:30 **Valery Romanovsky** (Univerza v Mariboru): Invariants and time-reversibility in polynomial systems of ODEs

11:30–13:00 Lunch break (City tour to Stoczek cafeteria)

13:00–13:20 **Attila László Nagy**, **János Tóth** (BME TTK): Blow-up in stochastic kinetics

The usual stochastic model of chemical reactions endowed with some appropriately chosen kinetics attempts at describing the temporal behavior of discrete quantities of species involved. The talk focuses on the possible emergence of the blow-up phenomenon in such a model, i.e. when, roughly speaking, some species hits infinity in finite time. By exploring conditions in terms of kinetics that ensure or just exclude the blow-up we give some answers to this rarely tackled issue.

13:20–13:50 **Josef Hofbauer** (Universität Wien): Planar S-systems

13:50–14:10 **Éva Valkó** (ELTE TTK): Investigation of the effect of correlated uncertain rate parameters via the calculation of global and local sensitivity indices

Applications of uncertainty methods for models with correlated parameters are essential to investigate chemical kinetics models. An extended global sensitivity analysis method and a local sensitivity analysis method for correlated parameters were compared for the case of the syngas-air combustion system.

14:10–14:40 Boros Balázs (Universität Wien): Weak reversibility implies existence of a positive steady state

<https://arxiv.org/pdf/1710.04732.pdf>

14:40–15:20 Gy. Lipták, K. M. Hangos, M. Pituk, G. Szederkényi: Stability of complex balanced kinetic systems with time delays

In this lecture we analyze a class of delayed kinetic systems derived from mass action type reaction network models. The time delayed positive stoichiometric compatibility classes and the notion of complex balanced time delayed kinetic systems are defined. The uniqueness of equilibria within the time delayed positive stoichiometric compatibility classes is also shown. Moreover, the semi-stability of the equilibrium solutions for complex balanced systems with arbitrary time delays is shown using an appropriate Lyapunov-Krasovskii functional and LaSalle's invariance principle. As a consequence, it can be shown that every positive complex balanced equilibrium solution is locally asymptotically stable relative to its positive stoichiometric compatibility class.

15:20–15:50 Tea break, coffee included

15:50–16:30 Lente Gábor (Pécsi Tudományegyetem): The reaction-diffusion equation and its solution in two chemically relevant examples The reaction-diffusion equation is a semi-linear parabolic partial differential equation, which is used to describe the dependence of the concentrations of chemical species as a function of time and spatial coordinates in non-homogeneous systems. The lecture will present two examples of the use of this equation in systems that are often employed to gain experimental information on fast processes in chemical kinetics: the typical setup of stopped-flow and laser flash photolysis instruments. Some possibilities for obtaining analytical solutions will be discussed and also the common difficulties of numerical methods will be highlighted.

Part of it has been published here [10.1021/acs.jpca.7b00443](https://doi.org/10.1021/acs.jpca.7b00443)

16:30–16:50 J. Tóth, A. L. Nagy (BME TTK): Extent of reactions: initial studies

The concept of reaction extent introduced more than 80 years ago has until now escaped a systematic investigation. We investigate possible alternative definitions, existence, uniqueness, blow up, periodicity and stationary points. We pose an inverse problem as a purely algebraic problem.

16:50–17:00 Closing gala, summary, plans, outlook, discussion

17:00–24:00 Conference dinner (individual), as, where and when you like

Everyone interested is welcome.

János Tóth, local organizing committee