Final Report
Physically inspired control and diagnosis of nonlinear dynamic systems

During this OTKA project we have developed novel approaches, tools and techniques to explore the physical characteristics of nonlinear systems in order to design advanced methods for their dynamic analysis, control design and diagnosis.

Research directions
We have organized the problems to be investigated into four work packages:

WP1. Structure based analysis and control of nonlinear compartmental systems
WP2. Entropy-inspired Lyapunov functions and their use for analysis and control of generalized positive polynomial systems
WP3. Scheduling and diagnosis of discrete event systems based on following event sequences
WP4. Optimal operation of energy systems

The achieved research results are presented in the order of the work packages (WPs) of our Research Plan.

It is important to note that the full manuscripts of the referred published papers are available from the web-page of our group

http://daedalus.scl.sztaki.hu/PCRG/PCRG_publist_ISO.html

WP1. Structure based analysis and control of nonlinear compartmental systems

An important special class of nonlinear compartmental systems, the class of kinetic systems and its generalizations have been investigated, because these systems have a well defined structure that can be characterized using graphs.

Realizations An algorithm was developed to determine all possible structurally different linearly conjugate realizations of a given kinetic polynomial system. The solution is based on the iterative search for constrained dense realizations using linear programming. The correctness of the algorithm was proved, and possibilities of a parallel implementation were discussed [2].

A computation-oriented representation of uncertain kinetic systems was studied. It was assumed that the monomial coefficients of the ODEs belong to a polytopic set, which defines a set of dynamical systems for an uncertain model. An optimization-based computation model was proposed for the structural analysis of uncertain models. It was shown that the so-called dense realization containing the maximal number of reactions (directed edges) is computable in polynomial time, and it forms a superstructure among all the possible reaction graphs corresponding to an uncertain kinetic model, assuming a fixed set of complexes. An algorithm was also proposed to compute all possible reaction graph structures for an uncertain kinetic model [3].

Structure and realizations of generalized polynomial systems We have generalized the chemical reaction network (CRN) theory to the case of positive real exponents. It has been shown that several results of CRN theory carry over to the case of generalized mass action kinetics. It is known, however, that the most important properties of CRNs, including their deficiency, reversibility and balancing, are realization-dependent. Using model transformations a method is proposed for embedding the temperature dependent CRN models extended with energy balance into the class of generalized CRNs with positive real exponents. The embedding increases the state variables by two new ones with a nonlinear algebraic equation between them [16].

The class of generalized positive systems with rational functions in their right-hand sides were investigated. We have shown that the model form of a wide class of kinetic systems with rational terms in the reaction rates is invariant under a positive linear diagonal transformation. Thus, the concept of linear conjugacy defined originally for mass action systems was extended to rational biochemical models.

The generalized Kirchhoff matrix and the kinetic weighting matrix of the linearly conjugate models were given as functions of the computed transformation parameters. It was shown through the illustrative examples that the dense realization of a linearly conjugate rational model may contain more reactions than that of a dynamically equivalent one due to the additional degrees of freedom introduced by the linear transformation. The proposed matrix-based representation is suitable for the computational search of preferred graph structures corresponding to linearly conjugate realizations of rational kinetic models [8].

The kinetic realization problem of nonnegative delayed polynomial systems was investigated, where we assigned a chemical reaction network structure to a set of delayed polynomial differential equations, that realizes its dynamics. We showed that similarly to the non- delayed case, this problem is generally non-uniquely solvable. We extended existing results for the realization of non-delayed models by proposing an algorithm to build delayed realizations and proving that the so-called dense realization defines a superstructure in the delayed case, too [33].

WP2. Entropy-inspired Lyapunov functions and their use for analysis and control of generalized positive polynomial systems

Positive polynomial and quasi-polynomial systems possess a general logarithmic Lyapunov function that originates in the entropy function of kinetic systems. This Lyapunov function candidate enables to develop computationally effective ways of analysing stability and design feedback controllers for this important nonlinear system class.

Domain of attraction A novel method for computing a bounded estimate of the domain of attraction (DOA) of locally asymptotically stable uncertain rational nonlinear system models was proposed. Using linear fractional transformation and an additional simplification step, a novel automatic method for generating the rational terms to be considered in the Lyapunov function was given, which satisfies the requirements for system representation in [21]. Moreover, an algorithm for computing the so-called maximal annihilators was proposed, which contain the maximum number of linearly independent rows corresponding to a given feasibility domain. The proposed method effectively reduces the size of the resulting optimization problem without increasing the conservatism of the DOA computation (see [20]).

Delayed chemical reaction networks First, we have investigated chemical reaction network models with constant delays. The delayed models were approximated using the chain method known from the theory of differential equations. It was shown that important structural properties (such as reversibility and deficiency) of the approximated models are preserved in the approximating reaction networks. Moreover, the approximation gives rise to a Lyapunov-Krasovskii functional candidate for the original delayed systems that can be efficiently used for stability analysis (see in [12]).

Thereafter, the time delayed positive stoichiometric compatibility classes were introduced and the notion of complex balanced time delayed kinetic systems was defined in [10]. We proved the uniqueness of equilibrium solutions within the time delayed positive stoichiometric compatibility classes for the type of delayed kinetic systems derived from mass action type reaction network models. In our main result we proved the semistability of the equilibrium solutions for complex balanced systems with arbitrary time delays using the above defined Lyapunov-Krasovskii functional and LaSalle's invariance principle. As a consequence, we obtained that every positive complex balanced equilibrium solution is locally asymptotically stable relative to its positive stoichiometric compatibility class.

The above methods have been generalized for chemical reaction network models with distributed time delays. First, we analyzed the possible origin of delays in CRN models. We have found that CRNs containing linear reaction chains with multiple joint complexes can be transformed to an equivalent reduced order delayed CRN model with distributed time delays. For this purpose, our earlier method for decomposing the chains of linear reactions with multiple joint complexes was used together with the "linear chain trick". An analytical expression for the kernel function of the distributed delay was also derived from the reaction rate coefficients of the linear reaction chains [9].

Stabilizing feedback design New computational methods were proposed to construct polynomial feedback controllers for the stabilization of polynomial systems with linear input structure around a positive equilibrium point. Using the theory of chemical reaction networks (CRNs) and previous results on dynamical equivalence, a complex balanced or weakly reversible zero deficiency closed loop realization was achieved by computing the gain matrix of a polynomial feedback using optimization. It was shown that the feedback resulting in a complex balanced closed loop system having a prescribed equilibrium point can be computed using linear programming (LP). The robust version of the problem, when a convex set of polynomial systems is given over which a stabilizing controller is searched for, was also solvable with an LP solver. The feedback computation for rendering a polynomial system to deficiency zero weakly reversible form can be solved in the mixed integer linear programming (MILP) framework. It was also shown that involving new monomials (complexes) into the feedback does not improve the solvability of the problems [13], [15].

Furthermore, a new stabilizing feedback design method was proposed for time delayed nonnegative polynomial systems with a linear input structure [11]. Using a polynomial state feedback, the open loop system was transformed into a complex balanced kinetic system that is known to be stable with a known Lyapunov-Krasovskii functional. The computation problem was solved through semidefinite programming exploiting the fact that the reaction graph structure and weighting of a kinetic polynomial system are non-unique.

A novel control approach has also been developed for a class of CRNs that are interconnected through a delayed convection network [17]. First, a control-oriented model was proposed for interconnected CRNs. Second, based on this model, a distributed control method was introduced which assures that each CRN can be driven into a desired fixed point (setpoint) independently of the delay in the convection network. The proposed algorithm was also augmented with a disturbance attenuation term to compensate the effect of unknown input disturbances on setpoint tracking performance. The control design applies the theory of passive systems and methods developed for multi-agent systems.

WP3. Scheduling and diagnosis of discrete event systems based on following event sequences

Discrete event system models are powerful ways of describing the causal structure underlying event sequences, so they can be used for developing event-based diagnostic methods.

Diagnosis using event sequences A model-free diagnostic algorithm was described in [32], that is based on clustering qualitative event sequences called traces. A sufficient number of training traces was used instead of an internal model to specify the faulty model of the system. The diagnosis consisted of two consequent phases. In the off-line training phase diagnostic clusters representing nominal and faulty behaviour were formed from the set of training traces, while the center of these clusters was stored. In the on-line diagnosis phase arbitrary unknown traces were compared with the cluster centres, in order to recognize the most probable nominal or faulty scenario for the trace. The effects of different mapping functions and different qualitative ranges on the clustering and therefore the diagnostic resolution of the method was compared and discussed.

Discrete diagnostic methods for electrical networks A new online diagnosis method of technological systems was proposed that is based on their qualitative colored Petri-net model. The proposed diagnosis method can also be used when more than one faults occur in the system and the faults evolve during the operation of the system. In order to make the diagnosis of complex technological systems computationally feasible, a structural decomposition method was introduced to reduce the size of their occurrence graphs and to make the diagnosis easier [22, 26].

Furthermore, a simple and effective colored Petri net (CPN) model was developed for a special type of electrical networks that describe local transformer areas, in order to detect and localize illegal loads that may be present. The model was decomposed to characteristic structural elements called feeders with one or two sources the computation of which can be performed independently and in parallel. The CPN

model allows to handle the interval-type uncertainties in the model in a transparent and effective way (see in [23]).

A model-based diagnostic method was proposed for detecting and isolating non-technical losses (illegal loads) in low voltage electrical grids of one transformer area. The proposed method uses a simple static linear model of the network and it is based on analysing the differences between the measured and model-predicted voltages. As a preliminary off-line step of the diagnosis, a powerful electrical decomposition method was proposed, which breaks down the overall network to subsystems with one feeder layout enabling to make the computation efficient. The proposed method is able to detect and localize multiple illegal loads, and the amount of the illegal consumption can also be estimated, see in [24] and [25].

WP4. Optimal operation of energy systems

Energy systems are of primary importance from the application point of view and present challenges for dynamic modelling, parameter estimation and optimal operation studies of nonlinear systems.

Smart inverters in electrical networks In order to effectively characterize voltage unbalance in electrical grids we proposed a new indicator of voltage deviation that may serve as a basis of analysis and compensation methods in this dimension of power quality. Firstly, a novel voltage norm capable of jointly indicating unbalance and under-voltage in a single value, afterwards a three phase unbalance reduction controller structure was given. As the third main result, the proposed controller structure was integrated with an optimization based control algorithm that uses asynchronous parallel pattern search as its engine. The proposed three phase inverter structure together with the control algorithm connected with a renewable source (photovoltaic panel or wind turbine) is capable of an asymmetric power injection or rerouting the energy flow to the grid so that the voltage unbalance decrease [18].

A current source inverter model has been developed in [19] that was constructed from six LTI models for the different switching modes. The overall model is in a piecewise affine form that supports the use of model predictive control. The model has been verified against engineering expectations and its open-loop performance shows that it is a promising basis of model predictive control structures [19].

Optimal operation of freezers A novel heuristic model-based optimal scheduling algorithm was proposed to operate heating and cooling type home appliances connected to smart grids where the price of the electrical energy is known in advance and temperature constraints are present. The accuracy and the computational properties of the proposed method were compared to the schedule generated by the MPT toolbox [5]. The algorithm works well with a relatively short prediction horizon using a fraction of the computing time needed for the MPT-based method. The robustness of the algorithm was also investigated with respect to the load of the refrigerator [6, 4].

Model-based diagnosis of electrical batteries A novel experiment design method for parameter estimation of a lithium ion battery was proposed in [27]. A simple equivalent electrical circuit model was used for this purpose that is nonlinear both in its variables and in its parameters. This method can be used for the estimation of the temperature dependence of the battery parameters in [28].

Monographic work

As a summary of our results in the area of polynomial dynamic models, a book entitled "Analysis and Control of Polynomial Dynamic Models with Biological Applications" [30] has been published by Academic Press, London.

As a summary of our results in the area of reaction kinetic networks, an invited book chapter
Szederkényi, G., Hangos, K. M.: "Chemical Reaction Networks as General Representations of Positive Polynomial Systems" [29] In: Reedijk, J. (szerk.) Reference Module in Chemistry, Molecular Sciences and Chemical Engineering Waltham (MA), USA Elsevier Inc, (2019) pp. 1-14. , 14 p.
has been published.

PhD students and their achievements

Our PhD students and PhD candidates were active members of the research team. The following list summarizes their achievements possibly including the data of their defended PhD thesis.

- **Attila Gábor**: Doctoral School of Information Science and Technology University of Pannonia
  He defended his PhD thesis entitled "Model analysis and parameter estimation in biochemical reaction networks" [7] in 2017 under the supervision of K.M. Hangos.
- **Attila Tóth**: Doctoral School of Information Science and Technology University of Pannonia
  He defended his PhD thesis entitled "Event based diagnosis of process systems" [31] in 2017 under the supervision of K.M. Hangos.
- **György Lipták**: Doctoral School of Information Science and Technology University of Pannonia
  He defended his PhD thesis entitled "Analysis and control of nonnegative polynomial systems" [14] in 2018 under the joint supervision of K.M. Hangos and G. Szederkényi.
- **Bernadett Ács**: Roska TamÃąs Doctoral School of Sciences and Technology, PÃązmÃąny PÃľter Catholic University
  She defended her PhD thesis entitled "Structural analysis of biochemically motivated nonlinear systems" [1] in 2018 under the supervision of G. Szederkényi.
- **Roland Bálint**: Doctoral School of Information Science and Technology University of Pannonia
  He is now a PhD candidate working on his thesis, he has fulfilled all of the publication requirements of the doctoral school under the supervision of A. Magyar.
- **Richard Neukirchner**: Doctoral School of Information Science and Technology University of Pannonia
  He is now a PhD candidate working on his thesis, he has fulfilled all of the publication requirements of the doctoral school under the supervision of A. Magyar.
- **Anna Pózna**: Doctoral School of Information Science and Technology University of Pannonia
  She is now a PhD candidate working on his thesis, she has fulfilled all of the publication requirements of the doctoral school under the joint supervision of K.M. Hangos and M. Gerzson.

References

[1] B. Ács. *Structural analysis of biochemically motivated nonlinear systems*. PhD thesis, Roska TamÃąs Doctoral School of Sciences and Technology, PÃązmÃąny PÃľter Catholic University, 2018.

[2] B. Ács, G. Szederkényi, Zs. Tuza, and Z.A. Tuza. Computing all possible graph structures describing linearly conjugate realizations of kinetic systems. *Computer Physics Communications*, 204:11–20, 2016.

[3] G. Ács, G. Szlobodnyik, and G. Szederkényi. A computational approach to the structural analysis of uncertain kinetic systems. *Computer Physics Communications*, 228:83–95, 2018.

[4] R. Bálint, A. Fodor, K.M. Hangos, and A. Magyar. Cost-optimal model predictive scheduling of freezers. *Control Engineering Practice*, 80:61–69, 2018.

[5] R. Bálint and A. Magyar. Refrigerator optimal scheduling to minimize the cost of operation. *Hungarian Journal of Industry and Chemistry*, 44(2):99–104, 2016.

[6] R. Bálint, A. Magyar, and K.M. Hangos. Cost-optimal model predictive scheduling of home appliances. *IFAC-PapersOnLine*, 50(1):3344–3349, 2017.

[7] A. Gábor. *Model analysis and parameter estimation in biochemical reaction networks.* PhD thesis, Doctoral School of Information Sciences and Technology University of Pannonia, 2017.

[8] A. Gábor, K. M. Hangos, and G. Szederkényi. Linear conjugacy in biochemical reaction networks with rational reaction rates. *Journal of Mathematical Chemistry*, 54:1658–1676, 2016.

[9] G. Lipták and K. M. Hangos. Distributed delay model of the mckeithanâĂŹs network. *IFAC Papersonline*, 52-7:33–38, 2019.

[10] G. Lipták, K. M. Hangos, M. Pituk, and G. Szederkényi. Semistability of complex balanced kinetic systems with arbitrary time delays. *Systems and Control Letters*, 114:38–43, 2018.

[11] G. Lipták, K. M. Hangos, and G. Szederkényi. Stabilization of time delayed nonnegative polynomial systems through kinetic realization. In European Control Association (EUCA), editor, *18th European Control Conference (ECC)*, pages 3138–3143, 2019.

[12] G. Lipták, K.M. Hangos, and G. Szederkényi. Approximation of delayed chemical reaction networks. *Reaction Kinetics, Mechanisms and Catalysis*, 123(2):403–419, 2018.

[13] G. Lipták, G. Szederkényi, and K. M. Hangos. Computing zero deficiency realizations of kinetic systems. *Systems and Control Letters*, 81:24–30, 2015.

[14] Gy. Lipták. *Analysis and control of nonnegative polynomial systems.* PhD thesis, Doctoral School of Information Science and Technology University of Pannonia, 2018.

[15] Gy. Lipták, A. Magyar, and K. M. Hangos. LQ control of Lotka-Volterra systems based on their locally linearized dynamics. In *IFAC-PapersOnLine*, volume 49, pages 241–245. Elsevier BV, 2016.

[16] A. Magyar. Generalized mass action realizations of temperature dependent chemical reaction networks. *Reaction Kinetics, Mechanisms and Catalysis*, 126:587–600, 2019.

[17] L. Márton, G. Szederkényi, and K. M. Hangos. Distributed control of interconnected chemical reaction networks with delay. *Journal of Process Control*, 71:52–62, 2018.

[18] L. Neukirchner, P. Görbe, and A. Magyar. Voltage unbalance reduction in the domestic distribution area using asymmetric inverters. *Journal of Cleaner Production*, 142(4):1710–1720, 2017.

[19] L. Neukirchner and A. Magyar. Modelling a three-phase current source inverter. *Hungarian Journal of Industry and Chemistry*, 44(2):105–111, 2016.

[20] P. Polcz, Péni, and G. Szederkényi. Improved algorithm for computing the domain of attraction of rational nonlinear systems. *European Journal of Control*, 39:53–67, 2018.

[21] P. Polcz., T. Péni, and G. Szederkényi. Reduced linear fractional representation of nonlinear systems for stability analysis. *IFAC PapersOnline*, 51-2:37–42, 2018.

[22] A. Pózna, M. Gerzson, A. Leitold, and K. M. Hangos. Colored petri net based diagnosis of process systems. In *30th European Simulation and Modeling Conference, 26-28 October 2016, Las Palmas, Spain*, page 491, 2016.

[23] A.I Pózna, A. Fodor, M. Gerzson, and K.M. Hangos. Colored petri net model of electrical networks for diagnostic purposes. *IFAC-PapersOnLine*, 51(2):260–265, 2018.

[24] A.I Pózna, A. Fodor, and K.M. Hangos. Non-technical loss diagnosis in electrical networks with a radial layout. *Hungarian Journal of Industry and Chemistry*, 47(1):3–9, 2018.

[25] A.I Pózna, A. Fodor, and K.M. Hangos. Model-based fault detection and isolation of non-technical losses in electrical networks. *Mathematical and Computer Modelling of Dynamical Systems*, 25(4):397–428, 2019.

[26] A.I. Pózna, M. Gerzson, A. Leitold, and K.M. Hangos. Diagnosis of technological systems based on the structural decomposition of their coloured petri net model. *Hungarian Journal of Industry and Chemistry*, 44(2):121–128, 2016.

[27] A.I. Pózna, K.M. Hangos, and A. Magyar. Design of experiments for battery aging estimation. *IFAC-PapersOnline*, 51(28):386–391, 2018.

[28] A.I. Pózna, K.M. Hangos, and A. Magyar. Temperature dependent parameter estimation of electrical vehicle batteries. *Energies*, 12(19):3755, 2019.

[29] G. Szederkényi and K.M. Hangos. Chemical reaction networks as general representations of positive polynomial systems. In J. Reedijk, editor, *Elsevier Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*. Elsevier Inc., Waltham, MA, 2019.

[30] G. Szederkényi, A. Magyar, and K.M. Hangos. *Analysis and control of polynomial dynamic models with biological applications*. Academic Press, London, 2018.

[31] A. Tóth. *Event based diagnosis of process systems*. PhD thesis, Doctoral School of Information Sciences and Technology, 2016.

[32] A. Tóth and K.M. Hangos. A diagnostic method based on clustering qualitative event sequences. *Computers & Chemical Engineering*, 95:58–70, dec 2016.

[33] M. Vághy, G. Szlobodnyik, and G. Szederkényi. Kinetic realization of delayed polynomial dynamical models. *IFAC PapersOnLine*, 2019.