

Kinetic realizations of delayed dynamical models

Mihály Vághy^{1*}, Gábor Szederkényi¹, Gergely Szlobodnyik¹

¹Pázmány Péter Catholic University

*E-mail: vaghy.mihaly.andras@hallgato.ppke.hu

Keywords: chemical reaction networks, mass-action kinetics, delayed kinetic systems, linear programming

The nonnegative system classes are important tools in modeling such space/time varying phenomena, where the state variables are naturally positive (e.g. biochemical processes, reaction networks, compartmental systems). In a control system view the kinetic nonnegative systems are so-called universal descriptors [1]. In engineering practice it is often necessary that the delays appearing in the operation of processes (e.g. signal propagation, material flow) are modeled appropriately in order to describe the dynamic behavior precisely [2].

This work presents new results on the kinetic realization of delayed polynomial dynamical systems. A necessary and sufficient condition for the realizability of such models is given. Moreover, an algorithm is proposed for computing the so-called canonical realization of delayed models. An optimization based framework is generalized for computing dense linearly conjugate realizations, and all of the linearly conjugate realizations of kinetic systems using a fixed set of complexes. To prove the correctness of the algorithms, it is shown that dense linearly conjugate delayed reaction network realizations form a unique superstructure among all linearly conjugate realizations. Examples from the literature are presented to illustrate the applicability of the algorithms.

Acknowledgments

Supported by the ÚNKP-18-1-I-PPKE-47 New National Excellence Program of the Ministry of Human Capacities

References

- [1] P. Érdi and J. Tóth, *Mathematical Models of Chemical Reactions. Theory and Applications of Deterministic and Stochastic Models*. Manchester, Princeton: Manchester University Press, Princeton University Press, 1989.
- [2] M. Roussel, “The use of delay differential equations in chemical kinetics,” *The journal of physical chemistry*, vol. 100, no. 96, pp. 8323–8330, 1996.