

PhD research topic proposal
BME, Doctoral School of Mathematics and Computer Science

Name of supervisor :

János Tóth

Degree:

CSc

Title of the topic:

Applications of algebraic methods in chemical reaction kinetics

Short description:

The mathematical models of chemical reaction kinetics (also applied in several fields of biology or chemical engineering) are systems of nonlinear differential equations, mainly with polynomial right hand sides. To obtain chemically relevant results on the stationary and the transient solutions of these models different branches of algebra are useful. Linear algebra is always present (in controllability and observability questions explicitly, in other areas in a less explicit way). Groebner bases are useful in determining the stationary solutions, Lie algebra is used in several ways. To reach the end of some calculations quantifier elimination methods are needed. Graph theory is also useful. Introduction into the field can be found in our recent book (Tóth, J.; Nagy, A. L., Papp, D.: Reaction Kinetics, Springer, 2018) where the interested applicant will also find a series of unsolved problems, or in Feinberg's book (Foundations of Chemical Reaction Network Theory, 2019, Springer). The solution of a nonempty subset (chosen together by the supervisor and the applicant) of these problems will be the topics of the thesis. The work is done in strong cooperation with researchers from other countries.

Requirements:

MSC degree in mathematics, chemistry, chemical engineering, informatics or physics. Experience in research, good knowledge in differential equations and algebra; friendly relationship with applications (chemistry, biology) and programming (Wolfram language preferred) is needed.

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