# Developing computational tools and mathematical models for reaction-advection-diffusion systems

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## Abstract

The doctoral dissertation focuses on the development of computational tools and mathematical models for reaction-advection-diffusion systems. The complexity of natural chemical, physical, and biological processes necessitates the creation of advanced mathematical models that allow for accurate simulation and analysis of these phenomena. The primary objective of the dissertation was to develop computational schemes that enable the analysis of complex chemical, physical, and biological processes. Special attention was given to modeling the phenomena of Liesegang pattern formation, explosive detonation, and cell population evolution. The work focuses on the application of numerical algorithms in three areas:

1. Modeling of Liesegang pattern formation (diffusion-aggregation-reaction system).
2. Modeling of explosive detonation and the propagation of a detonation wave (advection-reaction system).
3. Modeling of cell population and microorganism evolution (stochastic processes).

The dissertation develops algorithms that allow for the simulation of the aforementioned processes. Each of the models is based on appropriate mathematical equations that describe physical and chemical phenomena.

Modeling Liesegang Patterns: In this case, kinetic equations of chemical reactions, advection and diffusion equations, and the law of supersaturation were applied to describe the process of pattern formation in chemical processes. The simulations employed algorithms based on partial differential equations (PDEs) that allow for the prediction of pattern formation over time.

Modeling Detonation: The process of explosive detonation is based on complex physical equations, such as the ideal gas equation of state, Navier-Stokes equations, and the

Rankine-Hugoniot conditions. Numerical algorithms were applied to model the propagation of the detonation wave, describing changes in physical parameters over time. The simulation results were compared with experimental data.

Modeling Cell Population Evolution: The Gillespie algorithm was used to model stochastic processes in biology, such as mutations in cellular and microbial populations. Modifications to the algorithm were introduced in the dissertation, allowing for efficient modeling of large populations, encompassing even millions of cells. The results were also compared with the deterministic model and data from the TCGA (The Cancer Genome Atlas) database.

The results of the simulations conducted in the dissertation confirm the accuracy of the developed models and algorithms. The Liesegang pattern formation models yielded results consistent with the Matalon-Packter laws and literature data. The explosive detonation simulations showed a high degree of agreement with experimental results. The modeling of cell population evolution provided precise data on population development and mutations, which is of significant importance in cancer research.

The dissertation demonstrates that the application of advanced computational and numerical methods to model reaction-advection-diffusion processes allows for the precise representation of real phenomena. The developed algorithms make a significant contribution to the advancement of simulation tools that can be applied in both scientific research and industrial contexts, particularly in fields such as chemistry, physics, and biology. The modifications to the Gillespie algorithm open up new possibilities for modeling the development of large cell populations, which is relevant in cancer and other disease research.