**T14 – Investigations of nonlinear dynamical chemical phenomena**

Our investigations are concentrated on two main topics:

1. **Nonlinear reaction-diffusion systems.**

Nonlinear chemical systems in which diffusion of reagents is the unique transport process can be treated as minimal models with spatiotemporal patterns. Such systems are described by the nonlinear partial differential equations of the parabolic type (reaction-diffusion equations). For the one-variable one-dimensional (1D) reaction-diffusion model all possible spatiotemporal patterns have been described [1] whereas for two-variable systems the list of possible patterns is far to be completed even in 1D systems. Last time earlier unknown patterns have been found in a two-variable 1D model of excitable reaction-diffusion system [2-4]. An example of such patterns is shown in the Figure on which details of the spatiotemporal evolution of a reactant illustrating the first oscillon and fragment of the breathing periodical structure [4]. In the right down corner the traveling impulse is visible.

The same model, in two-dimensional system (2D) however, has been used to produce patterns illustrating some changes between 1D and 2D systems [5,6] and mimicking all capital letters of the Latin alphabet [7]

![Pattern Example](image)

It shall be stressed that the both pictures have been obtained with the same values of all parameters of the model.

**References**


2. **Influence of fluctuations on far from equilibrium chemical systems.**

Nonlinear dynamical systems often exhibit enhanced sensitivity to fluctuations. Stochastic deviations from deterministic dynamics can be particularly significant in systems close to
bifurcations, where fluctuations may induce effects that reach the macroscopic level. Bifurcations are turning points at which qualitative changes of features of deterministic dynamics are developed. Since a stochastic evolution is to some extent nondeterministic, it can be expected that a vicinity of bifurcation significantly influences the stochastic dynamics. Very rich nonlinear behavior like limit cycle oscillations, bistability and excitability can be observed in thermochemical systems [9,13]. We have studied stochastic effects in a thermochemical system close to the supercritical and subcritical Hopf bifurcations, related to different scenarios of the emergence of limit cycles. Using the master equation approach we obtained the fluctuation induced transitions of the system between the limit cycle and the stable focus. The distribution of the first passage time from the limit cycle to the stable focus exhibits a multi-peak form. Figure gives the distributions of first escape times from the basin of attraction of SLC to the basin of attraction of SF for different numbers N of molecules [11].

![Figure: Distributions of first escape times](image)

The effect of coherence resonance for return time to the focus has also been detected for mono- and bi-stable systems [11]. This kind of stochastic resonance appears if the control factor of the magnitude of fluctuations is either the size of the system [11,12] or the heat of the exothermic reaction [13]. Analytical results based on the Boltzmann equation have indicated that fluctuations can influence drastically the dynamics of far-from-equilibrium systems in which the distribution of particles energy is perturbed due to a chemical reaction. These results have been confirmed by microscopic simulations using the direct Monte Carlo method (DSMC). The combined effect of fluctuations and nonequilibrium distribution of energy change significantly the speed and width of the chemical wave front involving the autocatalytic reaction [14]. In the bistable system, nonequilibrium effect can reverse the property of mono-/bi-stability as compared to the unperturbed deterministic dynamics, proved by the fluctuation induced transition between the stable steady states observed in stochastic dynamics [15].

**References**