Pattern Formation and Chaotic Dynamics in a Cross-Flow Catalytic Converter with Kinetics of Detoxification of Exhaust Gases

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Heterogeneous catalytic reactions and catalytic reactors are known to exhibit complex dynamic behaviour. In the past three decades, significant progress in understanding this complexity has been made using the tools of nonlinear dynamics and advanced experimental methods. Nonetheless, theoretical predictions of pattern occurrence in various types of reactors including the fixed bed and cross-flow catalytic reactors are of great interest in understanding feasible dynamics in reactors used in applications.

In this contribution, the range of patterns occurring due to interaction of transport and reactions characteristic of the three-way catalytic converter (TWC) have been explored. We examined whether and how spatiotemporal structures such as spatially nonhomogeneous steady states and travelling waves are produced. Furthermore we found that the system displays a wide variety of chaotic spatiotemporal patterns, which were examined in detail.

Generally, heterogeneous reaction mechanisms include many positive and negative feedbacks therefore methods of stoichiometric network analysis (SNA) can be employed [1]. The SNA provides a natural way how to decompose the entire chemical network into elementary subnetworks and identify those among them that are potentially a source of nontrivial dynamical instabilities. The TWC reaction mechanism can be naturally decomposed according to reaction species into two independent subsystems [2]: the model combining oxidations of CO and C_2H_2, and the model of simultaneous CO oxidation and NO_x reduction. Even these models are capable to produce complex dynamical behaviour such as stable kinetic oscillations, multiplicity of steady states and hysteresis. The results of SNA for these subsystems can be used to interpret bifurcation diagrams of the two lumped parameter models [3]. Bifurcation diagrams usually display information about dynamical behaviour on a parametric plane. Further, we examine the dynamics in dependence on mass transport by diffusion or convection (or both).

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