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Spatiotemporal patterns in reaction–diffusion system of catalytic oxidation of CO and hydrocarbons

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Dynamical behaviour of catalytic oxidation of carbon monoxide and hydrocarbons in a catalytic converter can be in the simplest approximation described by a model of isothermal stirred flow-through reactor. When looking for an answer to which part of the mechanism is responsible for the nonlinear phenomena such as bistability of the steady states or the oscillatory behaviour, the theory of stoichiometric network analysis (SNA) has been used to analyze two major parts in a detailed mechanism of the overall reaction taking place in the converter – catalytic oxidation of CO and of hydrocarbons (exemplified by C_2H_2). By constructing the bifurcation diagram we can localize the areas in a parametric plane which can provide these nonlinear instabilities. Complex reaction kinetics is then coupled with transport processes in a tubular reactor with a cross-flow and nonlinear instabilities have been further examined as to what is their contribution to spatiotemporal patterns and waves in reaction-diffusion system. This approach leads to a refined classification of complex spatiotemporal dynamics based on that for subsystems possessing only reaction subnetworks displaying a specific type of chemical instability.