Pattern formation and chaotic dynamics in a three-way catalytic reactor with cross-flow

Martin Kohout[1], Otto Hadac[1], Jaromir Havlica[2], & Igor Schreiber[1]

[1] Department of Chemical Engineering, Center for Nonlinear Dynamics of Chemical and Biological Systems, Institute of Chemical Technology, Prague, Technicka 5, 166 28 Prague 6, Czech Republic,
[2] Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic, Rozvojova 135, 165 02 Prague 6, Czech Republic
kohoutm@vscht.cz

A three-way catalytic converter (TWC) is the most common reactor for detoxification of automobile exhaust gases. This catalytic reactor is typically operated with periodic variation of inlet oxygen concentration. In the TWC carbon monoxide, hydrocarbons and nitrogen oxides are transformed into carbon dioxide, nitrogen and water vapor. Dynamics of models describing this complex catalytic reaction set taking place in a cross-flow tubular reactor are examined.

We begin with a detailed kinetic model proposed for three-way catalytic converters. In an effort to relate resulting patterns to specific pathways in the mechanism we select two reaction subsystems combining CO oxidation with oxidation of C_2H_2 and with NO_x reduction. The ability of these two subsystems to generate nonlinear dynamical effects is examined first by neglecting transport phenomena and studying a lumped (CSTR) system with the use of stoichiometric network and bifurcation analysis.

Spatiotemporal behavior due to reaction kinetics combined with transport processes have been further studied in tubular reactor with cross-flow (TFR). Based on knowledge of the lumped dynamics, the observed spatiotemporal patterns are classified as phase waves, travelling front and pulse waves and chaotic spatiotemporal patterns. Their dependence on input parameters is systematically studied and their relation to different unstable reaction pathways is discussed.