251f Nonlinear Dynamics of Forced Catalytic Converters

Milos A. Marek, Petr Koci, Vladimir Nevoral, Matyas Schejbal, and Milan Kubicek

Typical three-way catalytic converter is operated as a forced system, where the inlet oxygen concentration varies with a frequency of approximately 1 Hz. The results of bifurcation analysis of the lumped approximate model of the three way catalytic conventer using the nonstationary reaction kinetics wil be described. The analysis predicted oscillations in the CO oxidation submodel based on nonstationary kinetics similarly as in the full nonstationary kinetic model of the TWC converter. The used reaction network has been investigated by stoichiometric network analysis [1]. Major unstable reaction subnetworks underlying oscillations in the CO and hydrocarbon oxidation have been identified. The nonlinear dynamics of CO oxidation in the lumped isothermal reactor model has been analyzed in detail. The constructed evolution diagram confirmed the existence of hysteresis and oscillations. It was found that in a certain range of the inlet oxygen concentrations there coexist low-and high-conversion stable stationary solutions. The coexistence of stable periodic solutions with stable stationary solutions was found to occur in another range of the inlet oxygen concentrations. Simulations of the model converter with periodically varying inlet oxygen concentrations revealed the existence of complex oeriodic and aperiodic regimes.Detailed analysis based on the use of continuation methods for analysis of periodically forced systems and computation of Lyapunov exponents revealed the existence of periodic, quasiperiodic and chaotic solutions. Arnold tongues in the parametric plane frequency - amplitude of the inlet oxygen concentration have been constructed and related to time-averaged outled conversions of CO. In the forced model of TWC converter it was found that the time averaged conversions of NOx depend strongly on the type of the inlet oxygen concentration forcing. [1]. P. Koci, V. Nevoral, M. Zahrubsky, M. Kubicek and M. Marek, Chem. Eng. Sci., 2004, 59, 5597-5605.