Time series analysis of an pH oscillatory chemical reaction

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We examine transition from periodic to chaotic oscillations experimentally observed in the continuous stirred tank reactor with the reaction of hydrogen peroxide, thiosulfate and sulfite in weakly acidic environment (HPTS) and presence of carbon dioxide. The HPTS reaction is an pH oscillator signifying that the hydrogen ions take part in the autocatalysis. Mixed-mode oscillations and chaos have been observed earlier but no detailed quantitative analysis of the degree of chaoticity were determined. The reaction is sensitive to the presence of carbon dioxide and a controlled inflow of this reactant has been chosen as the bifurcation parameter.

The measured time series of pH indicate simple periodic oscillations, mixed-mode oscillations of various degree of complexity and apparently chaotic oscillations with no distinct separation of amplitudes. We use SVD-based methods for reconstruction of phase portrait, noise reduction and determination of embedding dimension. There seem to be a few dozens of modes involved in building up the attractor and its geometry appears quite complex. We also calculate maximum Lyapunov exponent, which turns to positive values as the periodic mixed-mode regime transforms into chaos.

Building on an early version of a mechanism of this complex chemical reaction, we present an extended version and discuss its potential for reproducing the experiments using an approach based on stoichiometric network analysis.