Evaluation of the Nonlinear Frequency Response Method for the Hydrolysis of Acetic Anhydride

M. Felischak[1], D. Nikolic[2], M. Petkovska[2], C. Hamel[1,3], A. Seidel-Morgenstern[1,4]
[1]Otto-von-Guericke University Magdeburg, Dep. Chemical Process Engineering, Universitätsplatz 2, 39106 Magdeburg, Germany tel. +49 3916758128, e-mail: matthias.felischak@ovgu.de; [2]University of Belgrade, Serbia; [3]Anhalt University of Applied Sciences, Köthen, Germany; [4]Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany.

Dynamic operation can provide favorable equilibrium and kinetics, mass and heat transfer in chemical reactors, by an optimization of performance parameters. Usually fluctuations of inlet parameters are unwanted and can be even dangerous. Therefore detailed analysis of the system is needed to fully predict possible outcomes [1]. The method of nonlinear frequency response (NFR) attempts to predict the outcome of perturbation for the instructive input variables using nonlinear functions within the model equations. The aim of the derived models is the estimation of optimal frequencies and amplitudes for sinusoidal changes of the total inlet flow, concentration, temperature and the cooling temperature, as well as combinations of several of these inputs [2].

The NFR is an analytical method for the evaluation of periodically perturbed chemical reactors. Based on the concept of high order frequency response functions (FRFs) weakly nonlinear systems can be described. As an indicator for the performance of the forced periodic operation the value and sign of the non-periodic (DC) component of the outlet have to be analyzed, as shown in Fig. 1. This gives insight of possible improvements that can be implied by the input changes. By applying the NFR method the non-periodic term can be estimated for the modulation of a single and for multiple input parameters.

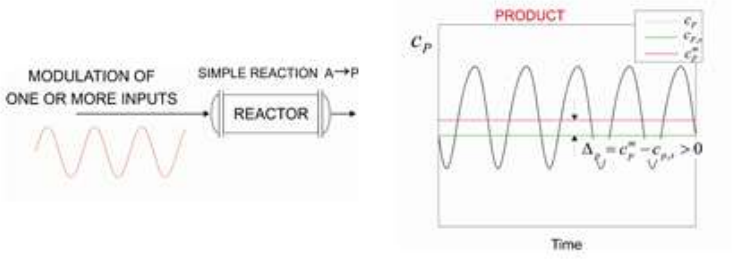

Fig 1: General Approach of the Nonlinear Frequency Response Function with sinusoidal change of the inlet parameters, resulting in a possible process intensification [3].

As a model reaction the hydrolysis of acetic anhydride in a continuously stirred tank reactor (CSTR) has been chosen. This exothermal reaction is investigated for the cases of separately and simultaneously modulated inlet concentrations and feed flow rates. For the experimental validation of predicted model-based results at first a verification and adjustment of the kinetic parameters is performed. Based on these results an optimal steady-state is calculated, which is used as an initial state of periodic operations. To estimate the performance of the reaction system mean values of the conversion of acetic anhydride and the yield of acetic acid are compared to the corresponding steady-state values of the reactor. Different forcing frequencies, input amplitudes and, for multiple input parameter, phase shift between them are investigated. The theoretical foundation as well as systematic exploration of the experimental possibilities will be presented.

[1] J.E. Bailey, Chemical Engineering Communications, 1 (1973) 111-124.
[2] P.L. Silveston, R.R. Hudgins, Periodic Operation of Chemical Reactors, ISBN: 978-0-12-391854-3.
[3] M. Petkovska, D. Nikolic, A. Markovic, A. Seidel-Morgenstern, Chemical Engineering Science, 65 (2010) 3632-3637.