Exploiting the Nonlinear Frequency Response Method to Evaluate the Potential of Forced Periodic Operation of Reactors

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Introduction

Forced periodic operation of chemical reactors possess significant potential to improve numerous performance criteria. The corresponding analysis of reaction systems and the estimation of the magnitude of possible performance improvements have occupied many researchers since the earlier explorations by Douglas and Rippin (1966), Horn and Lin (1967) and Bailey (1973). Theoretical problems related to identification and estimation of enhancement were typically analyzed evaluating suitable control criteria applying four major approaches described by Watanabe et al. (1981) and Parulekar (2003). However, there are hardly industrial applications of the promising concept and there is still a need in generally applicable methods for identifying and analyzing promising reaction systems.

New Approach

We suggest applying the nonlinear frequency response (NFR) method to predict the outcome of perturbing periodically one or several input variables. Applying the concept of higher order frequency response functions (FRFs) weakly nonlinear systems can be described analytically (Petkovska and Seidel-Morgenstern, 2013). Those systems contain a harmonic and a non-periodic (DC) term. As an indicator for the mean performance of the forced periodic operation the value and sign of the DC component of the outlet give insight up to which extent improvements can be expected by the forced input changes. Applying the NRF method the non-periodic

term can be efficiently estimated for the modulation of a single input and also for multiple inputs.

To demonstrate the strength of the theoretical concept the model of an adiabatic CSTR was analyzed considering reactions of different order. Estimates are provided for different frequencies of sinusoidal changes of the inlet composition, the total inlet flow and the feed temperature. It will be shown, that it is in particular attractive to perturb simultaneously two input variables using an optimal phase shift, which can be determined using our method (Nikolic et al., 2015).

Experimental

To validate theoretical predictions we carried out experiments in a laboratory scale CSTR considering the hydrolysis of acetic anhydride as a test reaction. The performance of the reaction system was evaluated with respect to different objectives under various steady state conditions, including theoretically optimal ones, and for various types of single and binary input perturbations.

References

- Bailey, J.E. (1973), "Periodic Operation of Chemical Reactors: A Review", *Chem. Eng. Comm.*, 1, 111.
- Douglas, J.M. and Rippin, D.W.T. (1966), "Unsteady state process operation", *Chem. Eng. Sci.* 21, 1966, 305.
- Horn, F. J. M. and Lin, R. C. (1967). "Periodic processes: A variation approach", *Ind. Eng. Chem. Process Des. Dev.*, 6, 21.
- Nikolic D., Seidel-Morgenstern A., Petkovska M. (2015), "Nonlinear frequency response analysis of forced periodic operation of non-isothermal CSTR with simultaneous modulation of inlet concentration and temperature", *Chem. Eng. Sci.*, 137, 40.
- Parulekar, S.J. (2003), "Systematic performance analysis of continuous processes subject to multiple input cycling", *Chem. Eng. Sci.*, 58, 5173.
- Petkovska M., Seidel-Morgenstern A. (2013). "Evaluation of Periodic Processes", in: "Periodic Operation of Chemical Reactors",
 - Eds.: Silveston P.L., Hudgins R.R., Elsevier, Oxford, Chapter 14, 387-413.
- Watanabe, N., Onogi, K. and Matsubara, M. (1981), "Periodic control of continuous Stirred tank reactors-I. The π criterion and its application to isothermal cases", *Chem. Eng. Sci.*, 36, 809.