Evaluating the Potential of Forced Periodic Operations of Chemical Reactors - The Nonlinear Frequency Response Approach

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One way to achieve process intensification is to operate the process in a periodic way, by cycling one or more input variables, in order to obtain better average performance compared to the optimal steady-state operation. The source of the possible improvement lies in the process nonlinearity. Nevertheless, the improvement is obtained only in some cases, while in some others the periodic operation can result in deterioration.

Periodic operations of chemical reactors have been attracting attention of a number of research groups, since the pioneering works of, e.g., Douglas and Rippin [1] and Bailey [2]. A review of the recent research in this area can be found in a book by Silveston and Hudgins [3].

Testing whether a potential periodic process is favourable or unfavourable generally demands long and tedious experimental and/or numerical work. In this work we present an alternative approach, based on the nonlinear frequency response (NFR) analysis, which gives an approximate value of the average process performance directly, without numerical simulation. The method is applicable for stable, weakly nonlinear systems.

The mathematical foundations of the nonlinear frequency response method are based on Volterra series and the resulting concept of higher order frequency response functions (FRFs). The method is based on the following facts:

- Frequency response (periodic steady-state) of a weakly nonlinear system consists of a non-periodic (DC) term, the basic and indefinite number of higher harmonics, where only the non-periodic term is responsible for the average process performance during the periodic process.

- The nonlinear model of a weakly nonlinear system can be replaced with an indefinite sequence of frequency response functions of different orders.
- The non-periodic term of the frequency response can be approximated by its dominant term which is proportional to the asymmetrical second order FRF.

The nonlinear frequency response method has been applied for analysis of periodic operations of isothermal and non-isothermal CSTRs with simple reaction mechanisms. Modulation strategies with one modulated input and with simultaneous modulation of two inputs have been analysed. Periodic operations with sinusoidal or any other shape of periodic modulation can be considered. The NFR method gives answers to the following questions:

- Is it possible to improve the performance of a particular reactor by periodic modulation of one or more inputs?
- Which range of frequencies of the input modulation(s) should be used in order to get the improvement?
- If simultaneous modulation of two inputs is used, what is the optimal phase difference between them?
- Are there some optimal values of the input amplitudes that should be used, and if there are, how to determine them?
- What is the approximate extent of the performance improvement for a particular periodic operation, for a chosen set of forcing parameters (frequency, amplitude(s) and phase difference).

The purpose of the method is fast evaluation of periodic operations, with the aim of selecting the cases and conditions which have a potential for improvement and are, therefore, worth of further, detailed numerical and experimental investigation.

References

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[3] Silveston P.L. and Hudgins R.R. (editors) (2013) Periodic Operations of Reactors, Bitherworth-Heineman (Elsevier)