Evaluation of possible performance improvement through periodic operation for the reaction of acetic acid anhydride hydrolysis – Nonlinear Frequency Response Approach

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Abstract

The nonlinear frequency response (NFR) method is a relatively new, fast and easy, analytical method for evaluating the performance of forced periodically operated chemical reactors. The method has been introduced in our previous publications. It is based on the concept of higher order frequency response functions (FRFs), which is applicable for weakly nonlinear systems. Frequency response of a weakly nonlinear system, in addition to the basic harmonic, contains a non-periodic (DC) term and, theoretically, an infinite sequence of higher harmonics. The DC component of the output is responsible for the average performance of the periodically operated reactor, and its sign and value define whether, and to which extent, the periodic operation leads to process improvement. Using the NFR method, this DC component can be approximately estimated from a single asymmetrical second order FRF (for modulation of a single input) or from several single input and cross-FRFs (for multiple-input modulation). For the case of multiple modulated inputs, the optimal phase difference between the modulated inputs is easily estimated.

In this work, the NFR method is used for evaluation of a forced periodically operated adiabatic continuous stirred tank reactor (CSTR) in which an exothermal reaction of hydrolysis of acetic acid anhydride, giving acetic acid takes place. The analysis is performed for the cases when inlet concentration of the reactant and flow-rate of the feed stream are periodically modulated, separately or simultaneously. Optimization of the steady-state operation of the reactor is performed first, and periodic operations around that steady-state are considered. Periodic operations with sinusoidal and square wave modulations are analysed and compared to the optimal steady-state operation. Conversion of the reactant (acetic acid anhydride) and yield of the product (acetic acid) are used for comparison. The kinetic data used for the analysis were obtained from previous experimental investigation.

The possible increase the conversion and a yield are analyzed as functions of the forcing frequency, input amplitude(s) and, for two-input modulation, the phase difference between them. It was shown that modulation of the inlet concentration would cause slight process improvement, while modulation of the flow-rate would worsen the reactor performance. It was also shown that simultaneous modulation of the inlet concentration and flow-rate would cause significant improvements.

The purpose of this work is to perform a screening of the forcing parameters (number and choice of the modulated inputs, forcing frequency, amplitude(s) and phase shift) of the periodic operations that would maximize the reactant conversion and the product yield for the reaction of acetic acid anhydride hydrolysis. This screening is preparation stage for experimental investigation which will be performed next.