Forced Periodic Operation: Effect of shapes for two simultaneously imposed modulations

M. Felischak[1], D. Nikolic[2], M. Petkovska[2], C. Hamel[1,3], A. Seidel-Morgenstern[1,4]
[1]Otto-von-Guericke University Magdeburg, 39106 Magdeburg, Germany; [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.
Corresponding author: matthias.felischak@ovgu.de

Introduction

The classical design of continuous chemical reactors exploits steady-state operation, which is optimized and maintained by appropriate control systems. Nevertheless, it is well-known that the reactor performance can be enhanced by applying periodic regimes, like forced modulations of input parameters [1,2].

The identification and evaluation of suitable periodic operation conditions is challenging. One approach that can be used is based on nonlinear frequency response (NFR) analysis [3]. The focus of this work is the experimental analysis of shapes for two simultaneously imposed modulations (sinusoidal and square) in comparison to results predicted by the NFR method. The acetic anhydride hydrolysis was studied in an adiabatic CSTR exploiting a periodic operation mode, which was found to be superior to the corresponding steady-state operation.

Theoretical Method

The Nonlinear Frequency Response (NFR) method is fast and easy to apply analytical method, capable of predicting the performance of forced periodically operated chemical reactors. Frequency response functions (FRF) of a weakly nonlinear system, in addition to the basic harmonic, contain a non-periodic (DC) term and an infinite sequence of higher harmonics [3]. The DC component of the output is directly linked to the average performance of the periodically operated reactor. The sign and value of the DC component define whether, and to which extent, the periodic operation leads to process improvement. Using the NFR method, this DC component can be approximated. For the case of multiple input variables modulated simultaneously the optimal phase difference between the modulated inputs can be directly determined [4,5]. The original method was developed for sinusoidal forcing functions. However, it can be extended to any shape of periodic input, such as simple square-waves (see Figure 1a) [6].

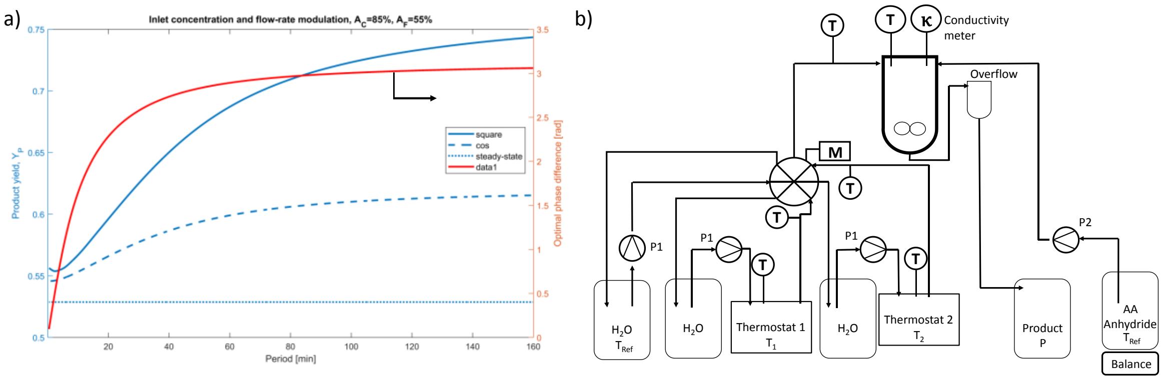

Figure 1: a) Comparison of yields for sinusoidal and square wave functions with optimal phase difference; b) Experimental setup for simultaneously modulating various inlet parameters.

Experimental Study

Based on theoretically developed FRFs for an adiabatic CSTR [5], the NFR analysis was performed for a model reaction, namely the acetic anhydride hydrolysis. Periodic operation around a steady-state were analyzed and compared to the optimal steady-state operation. Acetic acid yield was used for comparison, since it can be monitored easily using conductivity measurements. To verify the theoretical predictions of the NFR method, an experimental setup has been build (Figure 1b), which is capable to implement and control the input parameter modulation (frequency, amplitude and phase difference) for single or simultaneous modulation of the available parameters (flowrate, feed composition, inlet temperature).

Results

Preliminary experiments evaluated that the forced periodic operation is possible and reliable for both single and simultaneous modulations. The experimental investigations confirmed the predictions of NFR analysis, simultaneously modulating the inlet concentration and flowrate imposing a sinusoidal function. For properly chosen phase differences, it was possible to obtain beneficial reactor operation. Based on the evaluation of general inlet function shapes, in addition to harmonic inlets, also square waves were implemented. The application of the latter is even more promising, because the nonlinearities are more pronounced. Predicted mean reactor performance improvements are experimentally validated to evaluate the potential of both the concept and the NFR method as a predictive tool.

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