FREQUENCY RESPONSE ANALYSIS AS A TOOL FOR FAST EVALUATION OF PERIODIC OPERATIONS. CASE STUDY: A HETEROGENEOUS CATALYTIC REACTOR

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Abstract

One way to achieve process intensification is to operate the process in a periodic way, 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 be unfavourable.

Testing whether a potential periodic process is favourable or unfavourable generally demands long and tedious experimental and/or numerical work. This paper presents a new, fast and easy method for this testing, based on the Volterra series approach, nonlinear frequency response and the concept of higher order frequency response functions.

Without going into details, let us just remind that the frequency response of a nonlinear system, in addition to the basic harmonic, contains a non-periodic (DC) term, and an indefinite sequence of higher harmonics:

$$x = x_s + A\cos(\omega t) \xrightarrow[t\to\infty]{} y = y_s + y_{DC} + B_I\cos(\omega t + \varphi_I) + B_{II}\cos(2\omega t + \varphi_{II}) + \cdots$$

On the other hand, any nonlinear model with polynomial nonlinearity (**G**), can be replaced by an indefinite sequence of frequency response functions of different orders ($G_1(\omega)$, $G_2(\omega_1,\omega_2)$, $G_3(\omega_1,\omega_2,\omega_3)$,…), which are directly related to the DC component and different harmonics of the response. The DC component, which is responsible for the average performance of the periodic process, has a dominant term which is proportional to the asymmetrical second order function $G_2(\omega,-\omega)$:

$$y_{DC} = 2(A/2)^2 G_2(\omega,-\omega) + 6(A/2)^4 G_4(\omega,\omega,-\omega,-\omega) + \cdots$$

In principle, the sign of the asymmetrical second order function $G_2(\omega,-\omega)$ defines the sign of the DC component, and, accordingly, whether the periodic operation is favourable or unfavourable. In that way, in order to decide on the favourability of a particular periodic operation, it is enough to derive and analyse the function $G_2(\omega,-\omega)$.

In this work the method is applied to analysis of periodic reactor operation for a simple heterogeneous kinetic mechanism and for modulation of the input concentration. The analysis is performed for two reactor types: CSTR and PFTR. It shows that the answer whether the periodic operation is favourable or not, depends both on the reaction order and on the shape of the adsorption isotherm.

Approximate estimation of the average performance of the periodically operated process, is also illustrated. All mathematical operations are performed in the complex domain, using just complex algebra, instead of long and tedious numerical integration.