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Comparison of possible improvements of periodically operated adiabatic CSTR with inlet concentration modulation for different shapes of the forcing function

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Introduction

Forced periodic operations

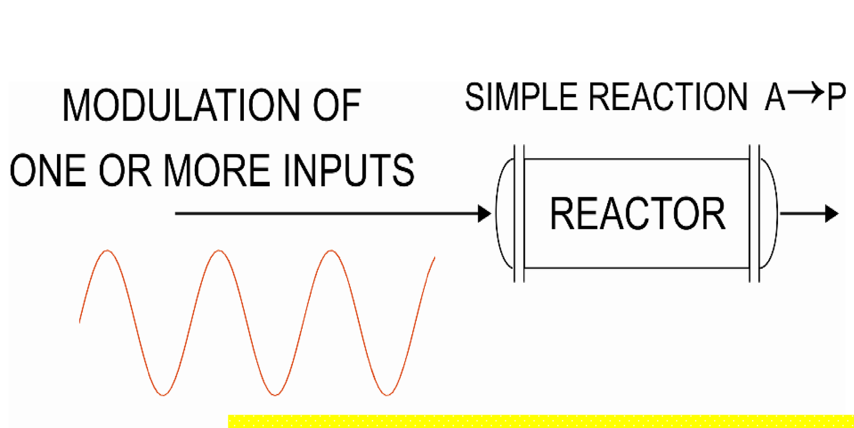
- One aspect of Process Intensification
- In some cases, the process performance can be enhanced by periodic modulation of some inputs around a chosen steady-state (result of the system nonlinearity)

Nonlinear Frequency Response Method

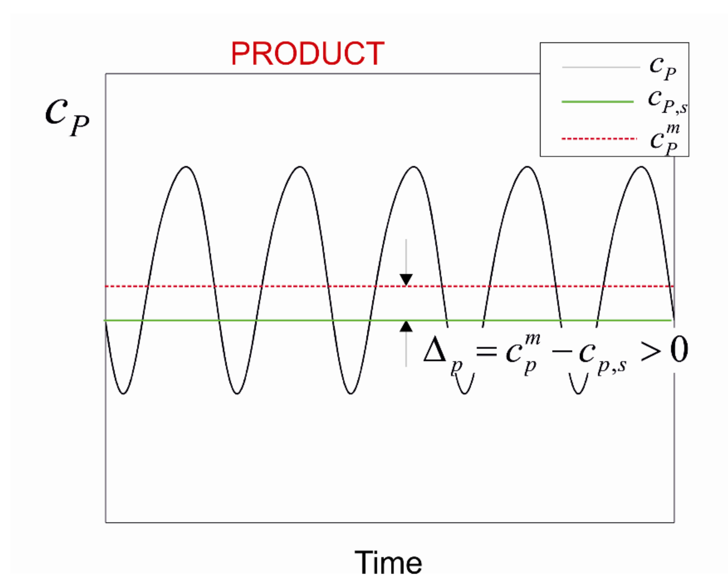
- Frequency response of a stable weakly nonlinear system is defined by a set of Frequency Response Functions (FRFs) of the first, second, third, … order
- The FR consists of indefinite number of harmonics and a non-periodic term

$$y = y_{DC} + B_I \cos(\omega t + \varphi_I) + B_{II} \cos(2\omega t + \varphi_{II}) + B_{III} \cos(3\omega t + \varphi_{III}) + \cdots$$

- y_{DC} – *the non-periodic term* – responsible for average performance of the periodic process – defines the process improvement through periodic operation ($\Delta \equiv y_{DC}$)
- **NFR method:** y_{DC} – *non-periodic term* proportional to $G_2(\omega,-\omega)$ – the asymmetrical second order (ASO) FRF



$$y_{DC} \approx 2(A/2)^2 G_2(\omega,-\omega)$$



General Input Waveform

Input modulation *X* of a general waveform

- Any periodic function can be represented as an infinite sum of harmonic functions, i.e. as a Fourier series.
- For practical applications, approximation with only the first *K* harmonics can be used

$$X(\tau) = \sum_{k=-\infty}^{\infty} \frac{A_k}{2} e^{jk\omega\tau}$$

DC component of the output *Y*

$$Y_{DC} \approx \sum_{k=-\infty}^{\infty} \left(\frac{A_k}{2}\right)^2 G_2(k\omega,-k\omega)$$

$G_2(k\omega,-k\omega)$ ASO FRF corresponding to the *k*-th harmonic of the input (correlating the output *Y* to input *X*)

DC Components for Different Shapes of the Input

Input modulation	DC component of output Y
Square-wave	$2\left(\frac{2A}{\pi}\right)^2 \sum_{k=1,3,5,\ldots}^{K} \left(\frac{1}{k}\right)^2 G_2(k\omega,-k\omega)$
Triangle	$2\left(\frac{4A}{\pi^2}\right)^2 \sum_{k=1,3,5\ldots}^{K} \left(\frac{(-1)^{\frac{k-1}{2}}}{k^2}\right)^2 G_2(k\omega,-k\omega)$
Saw-tooth	$2\left(\frac{A}{\pi}\right)^2 \sum_{k=1,2,3,\ldots}^{K} \frac{(-1)^{2k}}{k^2} G_2(k\omega,-k\omega)$

A - nominal amplitude
ω - forcing frequency
τ - time

Case Study – Adiabatic CSTR

Simple, irreversible, liquid homogeneous *n*-th order chemical reaction, $A \longrightarrow \nu_P P$, with a rate law $r = k_o e^{-\frac{E_A}{RT}} c_A^n$

Input: Inlet concentration of the reactant (C_{Ai})
Output: Outlet product concentration (C_P)
Yield of product $Y_{P,po} = Y_{P,s}(1 + C_{P,DC})$
Relative change of the product yield $\Delta Y_P = C_{P,DC}$

Asymmetrical second order FRF

$$G_2(\omega,-\omega) = \frac{(1+\alpha)^2}{2B_{ps}} \times \frac{\Lambda}{(\omega^2+1)(\omega^2+B_{ps}^2)}$$

Auxiliary parameters

$$\Lambda = n(n-1)\omega^2 + n^2(1-2\beta^2\gamma) - n(1+\beta\gamma)^2$$

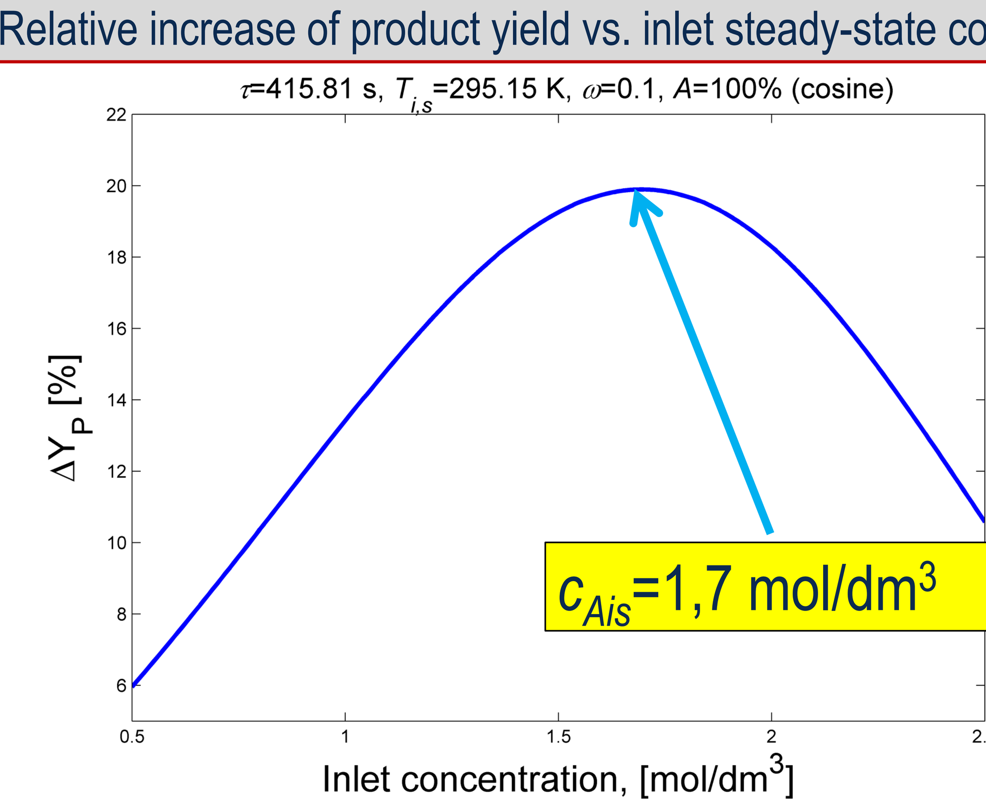
$$\alpha = k_o e^{-\frac{E_A}{RT_s}} c_{A,s}^{n-1} \frac{V}{F_s}, \beta = \frac{\Delta H_R k_o e^{-\frac{E_A}{RT_s}} c_{A,s}^n}{\rho \overline{c_P} T_s} \frac{V}{F_s}, \gamma = \frac{E_A}{RT_s}$$

Stability:

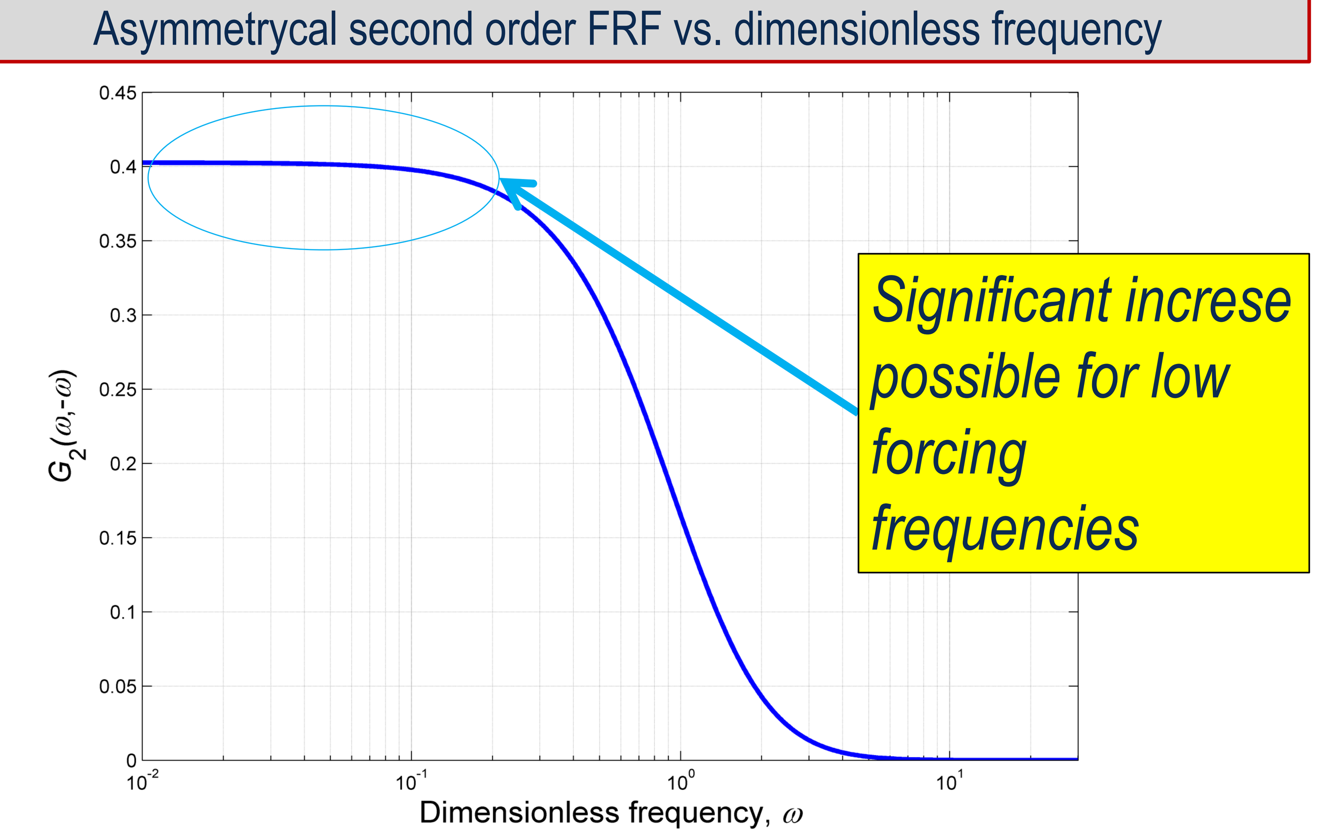
$$B_{ps} = 1 + n\alpha + \beta\gamma > 0$$

Parameters for reaction of hydrolysis of acetic acid anhydride (n=1, k_o =139390 1/s, E_A =44.350 kJ/mol , ΔH_R =-55.5 kJ/mol, $\overline{\rho c_p}$ =4.186 kJ/(K dm³))

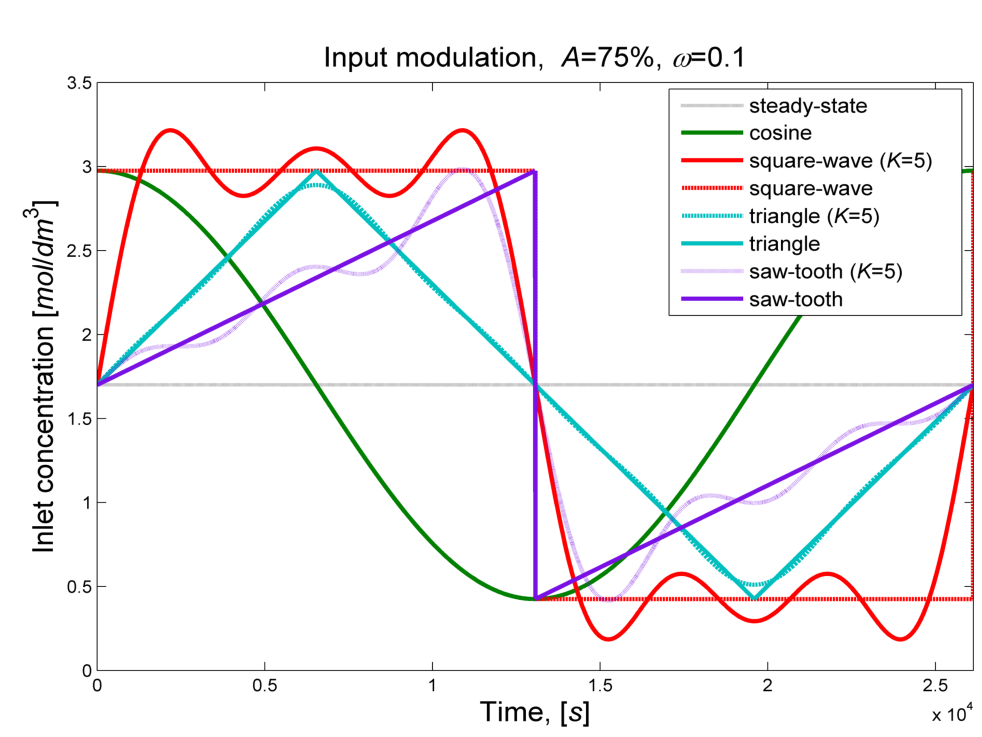
Relative increase of product yield vs. inlet steady-state concentration



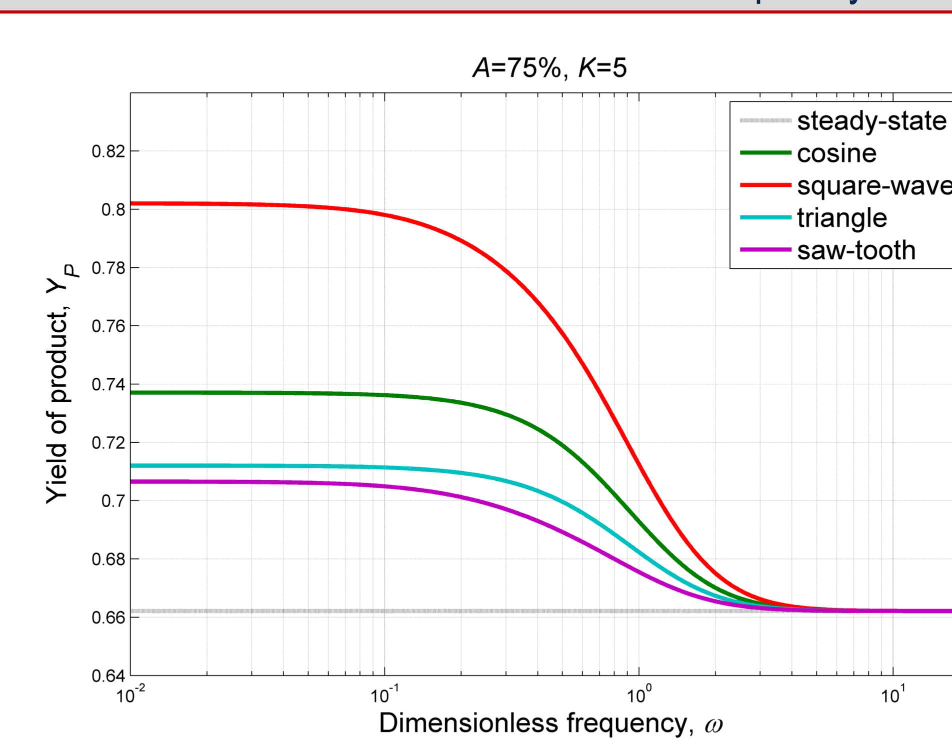
Asymmetrycal second order FRF vs. dimensionless frequency



Different shapes of inlet concentration modulation (approximated with *K*=5 harmonics)



Product yields for different shapes of input modulation and for steady-state vs. dimensionless frequency



Improvement possible for all shapes of forcing function!

Highest improvement for square-wave input modulation!

Comparison with numerical solution

Modulation	A [%]	K	$Y_{P,po}$(%) num	$Y_{P,po}$(%) NFR	δ_Y(%)
square-wave	25	1	67.73	67.55	-0.26
		3		67.68	-0.07
		5		67.72	-0.01
	75	1	78.25	78.22	-0.04
		3		79.44	1.52
		5		79.81	1.99

Excellent agreement!

Conclusions

- Estimation of possible improvements for different shapes of forcing function possible using the NFR method, just based on the second order approximation.

References

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