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Periodic optimization of a chemical reactor system using perturbation methods

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SUMMARY
A perturbation approach is presented to the periodic optimization problem of certain classes of nonlinear dynamical systems, for small-amplitude forcing functions, and within specific frequency ranges derived from Guardabassi's π-criterion. The procedure is illustrated by means of a classical example in chemical engineering, involving the optimal periodic operation of a continuous stirred tank reactor, in which two parallel reactions take place. The analysis is performed at cycling frequencies slightly above the minimum frequency, where, according to the π-criterion, performance improvement by cycling becomes possible. The per cent production gains over the optimal stationary operation are evaluated, as a function of the amplitude and frequency of the oscillations allowed to exist in the system, and as a function of the process parameters. Also the characteristics of the control and state waveforms are analysed. Thus the existence and practical applicability are demonstrated of a mathematical relationship between the optimal periodic control problem, the π-criterion, and the theory of perturbations.

1. Introduction

Design techniques for industrial plants are usually aimed at operating the system at a suitable, eventually optimal, constant state. In recent years however, especially in the field of chemical engineering, an increasing interest has become apparent in the possibility of allowing the control of a process to be varied periodically. A collection of applications-oriented papers on this topic can be found in [1]. An introduction to the theory of optimal periodic control is provided in [2, 3]. Papers in the area of periodic optimization of continuous systems are often related to one of the following two important questions. First the basic problem is raised, under what conditions the optimal steady-state operation of a given plant can be improved by implementing a nonconstant periodic regime. Once this point has been settled, the question naturally arises, how the obtained information could be exploited, to approach the optimal periodic operation as closely as possible, in terms of the selected performance index. A powerful tool to investigate the first problem is a frequency condition, developed by Guardabassi and his coworkers [4], which is known as the π-criterion. It encompasses, or is connected to, some earlier, more conservative results [5]. The second question is more difficult to answer. Necessary conditions for the optimal periodic operation of a continuous stationary dynamic system have been known for a relatively long time [5]. However, applying them to actually solve an optimal periodic control problem requires the explicit computation of periodic motions in the associated, normally nonlinear, Hamiltonian system. In the face of the extreme difficulty of solving this problem in general, considerable attention has been paid to the treatment of two limiting situations, that of very slow cycling (quasi-stationary operation), and that of very rapid cycling (relaxed operation). A thorough investigation of the relaxed operation of a continuous stirred tank reactor (CSTR) has been provided by Matsubara et al. [6]. These limiting modes have several obvious drawbacks. In no way do they explore the possibility of improving system performance by intentionally using the peculiar dynamics of the controlled system, since both relaxed and quasi-stationary control in fact eliminate the role of system dynamics. Moreover, high frequency control switchings, necessary to approximate a relaxed operation, may be difficult and costly to implement in practical situations, where such variables as temperatures or heat flow play the role of the driving function, which forces the system into oscillation.

Recently a possibility has been suggested to solve the optimal periodic control problem at frequencies, close to the critical frequencies which delimit the intervals where performance improvement may be realized, according to the π-criterion [7]. The method relies on classical perturbation techniques and provides only a partial and approximative solution to the optimal periodic control problem. In certain cases though, the supplied information may be useful. For example, if the π-criterion is satisfied in some bounded interval (ω_1, ω_2), then optimal periodic solutions may be obtained for frequencies, slightly larger than ω_1, and slightly smaller than ω_2. If ω_1 and ω_2 are not too far apart, and the computations are carried out to sufficient accuracy, a good estimate of the desired solutions may be found for all frequencies in (ω_1, ω_2). Another interesting case occurs when performance improvement is only possible for cycling frequencies larger than some lower bound ω_0. Increasing frequencies tend to increase the average speed of variation of the control force, as a function of time, and hence increase the difficulty of implementing this control. Therefore it is quite conceivable that in certain cases, from a technical point of view, a desirable mode of operation might be an optimal periodic control at some preselected frequency, slightly exceeding the minimum frequency where cycling becomes advantageous.

Of course, it must be stressed that restricting control frequencies to fall within the proximity of Guardabassi's critical frequencies, and also, requiring oscillation amplitudes to be small, are mathematical necessities for a perturbation technique to be valid, and these restrictions cannot be generally justified by practical considerations. Indeed, there is no general reason for presuming that technological or other practical engineering constraints would necessarily restrict the acceptable control frequencies and amplitudes in the indicated sense. However, since perturbation techniques seem to constitute the only available, general analytical tool for actually calculating oscillations in highly nonlinear systems, it seems to be a fair appraisal that such restricted results are the best that presently can be hoped for. Indeed, while the theories of relaxed and quasi-stationary periodic control are well-established today, no analytical, quantitative methods are available in the literature for the intermediate frequency range.

In the chemical engineering literature, a classical problem case of periodic optimization involves a periodically operated CSTR with two parallel reactions. Performance improvement by cycling is only possible for frequencies exceeding some minimum value. This example has been discussed by Horn and Lin [5], among many other investigators. In order to explain our approach, we shall intentionally reconsider this well known test case, such that, within the framework of the existing literature referring to it, the merits and shortcomings of the present method are clearly illustrated.

The relaxed operation of the CSTR with two parallel reactions was studied in [5], and also, to more detail, in [6]. In the present contribution, the optimal periodic operation of the same reactor system is analysed, but, with respect to the selected frequencies, the opposite extremum is considered of a relaxed control: The system is driven at frequencies, slightly larger than the minimum value at which performance improvement by cycling becomes possible. Also, in the performance index, oscillation amplitudes are penalized. As explained, pursueing such low amplitude and low frequency operation are both mathematical necessities for the perturbation method to apply, but, at the same time, these restrictions may, to some extent, be justified by practical considerations. The structure of the paper is as follows. First, for easy reference, a short review is given of the basic concept of finding solutions to an optimal periodic control problem using perturbation techniques. The formal problem statement for the considered application follows. After an outline of the computational procedure applied, the results are presented, yielding performance improvement and characteristics of the control and state waveforms, as functions of the amplitude and frequency of the state oscillation, and the system parameters. Two cases are considered, dealing with the parallel reaction of a linear and a second-order, resp. a linear and a third-order reaction.

2. Background

Consider an unconstrained optimal periodic control problem, with system equation

$$\dot{x} = f(x, u), \tag{1}$$

and performance index to be maximized,

$$J[u(.)] \triangleq \frac{1}{\tau}\int_0^\tau g(x, u)\,dt, \tag{2}$$

subject to the condition $x(0) = x(\tau)$. τ is a fixed positive constant. Define

$$h(x, u, \lambda) \triangleq g(x, u) + \lambda' f(x, u).$$

Let $\{x_0, u_0\}$ be optimal within the class of constant solutions of (1), and J_0 the corresponding value of (2). Then there exists a solution $\{x_0, u_0, \lambda_0\}$ of the system of algebraic equations

$$h_x(x_0, u_0, \lambda_0) = 0, \quad h_u(x_0, u_0, \lambda_0) = 0, \quad f(x_0, u_0) = 0. \tag{3}$$

Define

$$A \triangleq f_x(x_0, u_0), \quad B \triangleq f_u(x_0, u_0),$$

$$P \triangleq h_{xx}(x_0, u_0, \lambda_0), \quad Q \triangleq h_{xu}(x_0, u_0, \lambda_0), \quad R \triangleq h_{uu}(x_0, u_0, \lambda_0).$$

Letting $x = x_0 + \Delta x$, $u = u_0 + \Delta u$, (1) and (2) become

$$\Delta\dot{x} = A\Delta x + B\Delta u + \eta(\Delta x, \Delta u), \tag{1'}$$

$$J - J_0 = \frac{1}{\tau}\int_0^\tau [h(x, u, \lambda_0) - h(x_0, u_0, \lambda_0)]dt =$$

$$= \frac{1}{\tau}\int_0^\tau \left\{\frac{1}{2}\begin{bmatrix}\Delta x\\ \Delta u\end{bmatrix}'\begin{bmatrix}P & Q\\ Q' & R\end{bmatrix}\begin{bmatrix}\Delta x\\ \Delta u\end{bmatrix} + \zeta(\Delta x, \Delta u)\right\}dt. \qquad (2')$$

Here η is a second-order, and ζ a third-order expression in the components of Δx and Δu. Assume that A has no characteristic values on the imaginary axis, B has full rank and R is nonsingular. If there exists a continuous function $\Delta u(t)$, $0 \leqq t \leqq \tau$, for which (2′) is maximized, then $\Delta u(t)$, $\Delta x(t)$ and $p(t)$ satisfy the Hamiltonian system

$$\Delta\dot{x} = \frac{\partial H}{\partial p}, \quad (4.a); \qquad \dot{p} = -\frac{\partial H}{\partial \Delta x}, \quad (4.b); \qquad 0 = \frac{\partial H}{\partial \Delta u}, \quad (4.c);$$

where

$$H(\Delta x, \Delta u, p) \triangleq \frac{1}{2}\begin{bmatrix}\Delta x\\ \Delta u\end{bmatrix}'\begin{bmatrix}P & Q\\ Q' & R\end{bmatrix}\begin{bmatrix}\Delta x\\ \Delta u\end{bmatrix} + \zeta(\Delta x, \Delta u) + p'[A\Delta x + B\Delta u + \eta(\Delta x, \Delta u)], \qquad (5)$$

with the constraints $\Delta x(0) = \Delta x(\tau)$, $p(0) = p(\tau)$, hence, in view of the algebraic equation (4.c), $\Delta u(0) = \Delta u(\tau)$, [5]. After eliminating Δu, (4) takes the form

$$\dot{z} = Mz + \xi(z), \qquad (6)$$

$$M \triangleq \begin{bmatrix} A - BR^{-1}Q' & -BR^{-1}B' \\ -P + QR^{-1}Q' & -A' + QR^{-1}B'\end{bmatrix}, \qquad z \triangleq \begin{bmatrix}\Delta x\\ p\end{bmatrix}.$$

p is the costate vector of Δx, and ξ is a second-order expression in the components of z. By the π-criterion, a sufficient and locally necessary condition for the existence of a periodic operation with angular frequency ω, better than the optimal constant solution, is that $\Pi(\omega) \triangleq G'(-j\omega)PG(j\omega) + Q'G(j\omega) + G'(-j\omega)Q + R$, $G(s) \triangleq (sI - A)^{-1}B$, is partially positive [4]. Critical frequencies are called those frequencies ω_0 for which $\det \Pi(\omega_0) = 0$. If $\Pi(\omega)$ is partially positive for $\omega \in (\omega_0, \omega_b)$, and not partially positive for $\omega \in (\omega_a, \omega_0]$, then ω_0 is critical. In [7] it has been shown that if ω_0 is critical, then M has the characteristic values $\pm j\omega_0$. Now the substitution $z = \varepsilon\hat{z}$ transforms (6) into

$$\dot{\hat{z}} = M\hat{z} + \varepsilon\hat{\xi}(\hat{z}, \varepsilon), \qquad (7)$$

to which classical perturbation techniques can be applied for constructing periodic solutions with frequencies, close to the proper frequencies ω_0 of the unperturbed system, $\dot{\hat{z}} = M\hat{z}$. If an optimal admissible control with frequency ω exists, then it is a periodic solution of (7). This solution can be detected by solving the associated bifurcation equations, and computed by a method of successive approximations. The successive approximations converge to the desired solution if ε is sufficiently small, which implies that periodic solutions can be obtained with sufficiently small amplitudes, and frequencies, sufficiently close to ω_0.

3. System definition and problem statement

A CSTR is considered in which two parallel reactions, $A \to B$, of order α, and $A \to C$, of first order, take place. The reaction rates are given by the Arrhenius equations, $r_1 = h_1 \exp(-E_1/RT) \cdot C_A^\alpha$, and $r_2 = h_2 \exp(-E_2/RT) \cdot C_A$. Flow rate q and feed concentration C_{A0} are constant. The tank, of volume V, is temperature controlled. For this system the normalized dynamic equations read [5]:

$$\frac{dx_1}{dt} = -ux_1^\alpha - au^\rho x_1 - x_1 + 1, \tag{8.1}$$

$$\frac{dx_2}{dt} = ux_1^\alpha - x_2, \tag{8.2}$$

where the meaning of the symbols is the following:

$$x_1 = C_A/C_{A0}, \quad x_2 = C_B/C_{A0}, \quad t = qt_1/V, \quad u = (Vh_1/q)C_{A0}^{\alpha-1} \exp(-E_1/RT),$$

$$\rho = E_2/E_1, \quad a = (Vh_2/q)[(Vh_1/q)C_{A0}^{\alpha-1}]^{-\rho}$$

and t_1 representing real time. The objective is to maximize the average production of B by periodic optimization, while keeping oscillation amplitudes and frequencies within reasonable limits. As a performance index, let

$$J \triangleq \frac{1}{\tau} \int_0^\tau [x_2 - \theta(u - u_0)^4] dt \tag{9.1}$$

where u_0 is the optimal constant control, and $\theta > 0$ is a weighting coefficient. By an appropriate choice of θ, control fluctuations, hence also state fluctuations, can be effectively contained within preassigned boundaries. Integrating (8.2) and using the periodicity constraint $x_2(0) = x_2(\tau)$, shows that J can be written as

$$J = \frac{1}{\tau} \int_0^\tau [ux_1^\alpha - \theta(u - u_0)^4] dt, \tag{9.2}$$

where x_1 satisfies (8.1). Hence the problem is reduced to the periodic optimization of a first-order system.

As is well known [5], a static optimum $\{x_0, u_0\}$ exists if

$$\alpha\rho > 1, \tag{10}$$

which can be computed, together with the Lagrange multiplier λ_0, using (3). These equations yield

$$u_0 = [a(\alpha\rho - 1)]^{-1/\rho},$$

$$u_0 x_0^\alpha + (au_0^\rho + 1)x_0 - 1 = 0,$$

from which $x_0 > 0$ can be obtained, and

$$\lambda_0 = x_0^{\alpha-1}/(x_0^{\alpha-1} + a\rho u_0^{\rho-1}).$$

Then the static optimum equals

$$J_0 = u_0 x_0^\alpha.$$

Some further calculations reveal that

$$A = -\alpha u_0 x_0^{\alpha-1}/\lambda_0, \quad B = -x_0^\alpha/\lambda_0, \quad P = \alpha(\alpha-1)(1-\lambda_0)u_0 x_0^{\alpha-2},$$

$$Q = \alpha(1-\lambda_0)x_0^{\alpha-1} - a\rho\lambda_0 u_0^{\rho-1}, \quad R = -a\rho(\rho-1)\lambda_0 x_0 u_0^{\rho-2},$$

while $G(s) = B/(s-A)$ and $\Pi(\omega) = (PB^2 - 2QBA)/(\omega^2 + A^2) + R$. Since the static solution $\{x_0, u_0\}$ is optimal, $\Pi(0) < 0$, or

$$PB^2 - 2QBA + RA^2 < 0.$$

Then, by the π-criterion, the static optimum can be improved by cycling if $R > 0$, or

$$\rho < 1, \tag{11}$$

(cf. [5]), and the cycling frequency must exceed ω_0, defined by

$$\omega_0^2 = \frac{2QBA - PB^2 - RA^2}{R}.$$

ω_0 is independent of the weighting coefficient θ, because in the performance index (9.1) the fourth power of the control fluctuations was penalized (This would not be true if the second power had been used). The problem now consists in determining the optimal periodic regime for a given cycling frequency ω, slightly exceeding the critical frequency ω_0. The per cent production gain

$$\Gamma \triangleq \frac{1}{J_0\tau}\int_0^\tau (ux_1^\alpha - J_0)dt$$

$$= \frac{1}{J_0\tau}\int_0^\tau [h(x, u, \lambda_0) - h(x_0, u_0, \lambda_0) + \theta(u-u_0)^4]dt \tag{12}$$

will be evaluated as a function of the process parameters, and the characteristics of the control and state waveforms $u(t)$ and $x_1(t)$ will be analysed.

4. Computational procedure

In this section an outline is sketched of the successive computational steps involved, and the accuracy to which they have been carried out, in order to obtain the results presented below. The first step consists in determining the right hand sides of (1′) and (2′) with sufficient accuracy. This is done by expanding $f(x, u)$ and $h(x, u, \lambda_0)$ in Taylor series about the optimal constant solution $\{x_0, u_0\}$, yielding expressions of the form

$$\Delta\dot{x}_1 = A\Delta x_1 + B\Delta u + \sum_{i=0}^{2} \eta_{2,i}\Delta x_1^{2-i}\Delta u^i + \sum_{i=0}^{3} \eta_{3,i}\Delta x_1^{3-i}\Delta u^i, \tag{13}$$

$$h(x, u, \lambda_0) - h(x_0, u_0, \lambda_0) = \tfrac{1}{2}P\Delta x_1^2 + Q\Delta x_1 \Delta u + \tfrac{1}{2}R\Delta u^2 + \\ + \sum_{i=0}^{3} \zeta_{3,i}\Delta x_1^{3-i}\Delta u^i + \sum_{i=0}^{4} \zeta_{4,i}\Delta x_1^{4-i}\Delta u^i. \tag{14}$$

Expansions up to the third, resp. fourth order terms in (13) and (14) are necessary to compute the first term in the series expansion of Γ, which is proportional to the fourth power of the oscillation amplitudes (see below). Higher-order terms have been neglected. The coefficients appearing in the expansions are functions of the system parameters α, a and ρ. Note that $\zeta_{4,4}$ is the only coefficient which depends on θ. Subsequently the Hamiltonian H is constructed according to (5) and the equations (4.b–c) are derived, having the form

$$\dot{p} = -P\Delta x_1 - Q\Delta u + O^2(\Delta x_1, \Delta u, p) + O^3(\Delta x_1, \Delta u, p), \tag{15}$$

$$R\Delta u + Q\Delta x_1 + Bp = O^2(\Delta x_1, \Delta u, p) + O^3(\Delta x_1, \Delta u, p). \tag{16}$$

From (16), Δu must be obtained as a series expansion in Δx_1 and p. This is done by successive approximations, the first approximation being

$$\Delta u = -\frac{Q}{R}\Delta x_1 - \frac{B}{R}p. \tag{17}$$

Substituting (17) in the right hand side of (16) and neglecting third-order terms, yields the second approximation, $\Delta u = -(Q/R)\Delta x_1 - (B/R)p + \sum_{i=0}^{2} \psi_{2,i}\Delta x_1^{2-i}p^i$, and, proceeding in the same way, the desired result

$$\Delta u = -\frac{Q}{R}\Delta x_1 - \frac{B}{R}p + \sum_{i=0}^{2} \psi_{2,i}\Delta x_1^{2-i}p^i + \sum_{i=0}^{3} \psi_{3,i}\Delta x_1^{3-i}p^i \tag{18}$$

is found. Substituting (18) in (13) and (15) produces the system (6), with

$$M = \begin{bmatrix} A - BQ/R & -B^2/R \\ -P + Q^2/R & -A + QB/R \end{bmatrix},$$

and the components of the vector $\xi(z)$ having the form

$$\xi_j(z) = \sum_{i=0}^{2} \xi_{j,2,i}\Delta x_1^{2-i}p^i + \sum_{i=0}^{3} \xi_{j,3,i}\Delta x_1^{3-i}p^i, \quad j = 1, 2$$

M has the characteristic values $\pm j\omega_0$, as explained in section 2. After transforming (6) into (7) the desired periodic solutions can be obtained using a standard perturbation analysis [8], yielding results of the form

$$\Delta x_1 = R_0 \sin \omega t + R_0^2[\alpha_1 + \alpha_2 \sin(2\omega t + \phi_1)] + O(R_0^3), \tag{19}$$

$$\Delta u = \frac{\sqrt{\omega_0^2 + A^2}}{B} R_0 \sin\left[\omega t - \operatorname{arc\,tg}\left(\frac{\omega_0}{A}\right)\right] + R_0^2[\alpha_3 + \alpha_4 \sin(2\omega t + \phi_2)] + \\ + O(R_0^3), \tag{20}$$

$$\omega = \omega_0 + \alpha_5(\theta)R_0^2 + O(R_0^4), \tag{21}$$

$$\Gamma = \alpha_6(\theta)R_0^4 + O(R_0^6). \tag{22}$$

R_0 is proportional to ε. The coefficients α_1–α_4 and ϕ_1–ϕ_2 depend on the process parameters α, a and ρ, but not on θ; α_5 and α_6, however, depend on the process parameters and on θ. This means that the weighting coefficient in the performance index (9.1) only affects the frequency-amplitude relationship (21) of the optimal periodic operation and the per cent production gains (22), but has no direct effect on the form of the state and control functions (19) and (20), up to the second harmonics. These expressions only depend on θ implicitly, through the relation (21).

5. Results

As already stated, the process dynamics depend on the parameters α, a and ρ. In addition, the weighting coefficient θ was introduced in the performance index (9.1). α and ρ must satisfy the inequalities (10, 11), in order that there exists a static optimum which can be improved by cycling. This implies that the integer α must at least equal 2. A complete analysis of the production gains and the state and control waveforms, up to the second harmonics, has been carried out for the case $\alpha = 2$. The results for higher values of α, in particular for $\alpha = 3$, are quite analogous. Therefore merely a short discussion for the case $\alpha = 3$ has been included, without reproducing the numerical data. The choice of θ is determined by the size of the oscillations that can be allowed to exist in the system. A good measure for this size is R_0, the amplitude of the fundamental harmonic of the state waveform. Indeed, as will be shown below, the higher-order harmonics of $\Delta x_1(t)$ decrease in size rapidly, and the state oscillations are almost sinusoidal. For a given frequency ω and for given process parameters, θ is tied to R_0 by the relation (21). In all diagrams, the results have been represented as parametric curves, with R_0 as a variable parameter. For each choice of $\omega > \omega_0$ and R_0, the corresponding θ has been computed from (21), and the condition $\theta > 0$ has been checked. Remarkably enough, for $\theta = 0$, $\alpha_5(0)$ is consistently negative, which means that for $\theta = 0$ the Hamiltonian system (6) has no periodic solutions with $\omega > \omega_0$. Hence there exists no optimum if the oscillation amplitudes are not penalized. The influence of the parameter a on the results is small. For example, for $\alpha = 2$, $\rho = 0{,}8$, $R_0 = 0{,}1$ and $\omega = 1{,}25\omega_0$, the per cent production increase, as a function of a, varies according to the following table

a	Γ
0,5	1,2861%
1	1,2130%
1,5	1,1918%

Therefore, following Horn and Lin [5], a has been given the fixed value of $a = 1$ in all subsequent calculations. Then, only a single parameter, ρ, is left, which is confined to the interval $1/\alpha < \rho < 1$. Figure 1 displays the critical frequency ω_0, the optimal constant control u_0 and state x_0, and the corresponding production J_0, as functions of ρ, for $\alpha = 2$ and $a = 1$. ω_0 grows unbounded as ρ approaches its upper and lower limits. J_0 and u_0 decrease monotonically, and x_0 increases monotonically, for increasing ρ.

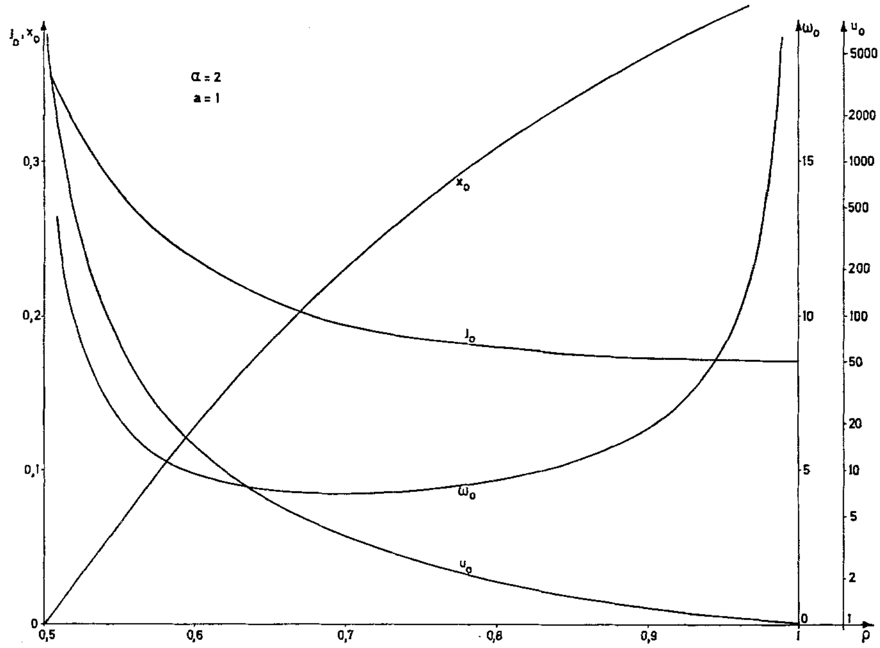


Figure 1. Critical frequency ω_0 and optimal constant values u_0, x_0 and J_0, as functions of ρ, and for $\alpha = 2$ and $a = 1$.

In Figure 2 the per cent production gains versus the coefficient ρ are shown for varying R_0, and for frequencies ω, selected at 10%, 25% and 40% above the critical frequency ω_0. The dotted line represents the points where the minimum value of the control function $u(t)$, during the cycle, becomes zero. Since $u(t)$ is a positive quantity, this line constitutes a physical upper bound for the production increases that can be obtained by the present analysis and the modes of operation resulting from it. The accuracy of the results decreases with increasing R_0 and increasing ω, for the reasons already explained. The maximum attainable Γ increases with increasing ω, the relationship being roughly proportional. This is to be expected, in view of the results in [5], where a hill-climbing search for the optimal periodic solution resulted in control functions with increasingly faster switchings, approaching a relaxed operation. Γ also increases with R_0. The increase is faster than linear, but slower than the fourth power relationship (22), which is valid for a constant θ. For a constant θ, ω grows with R_0, according to (21), hence inducing stronger increases of Γ than in the case where ω is kept constant.

In Figures 3–8, the control and state waveforms $\Delta u(t)$ and $\Delta x_1(t)$ have been analysed, up to the second harmonics. As already mentioned, the constant terms and the amplitudes and phase angles of the first and second harmonics do not depend on θ. Hence they can be studied as functions of the system parameters and of R_0, the results being valid for all ω. This is no longer true for the higher harmonics though. Since the higher harmonics also tend to decrease in size sharply (being proportional to increasingly higher powers of R_0), they have not been considered. Figure 3 shows the constant terms in $\Delta u(t)$ and $\Delta x_1(t)$, relative to the optimal constant values u_0 and x_0. Both ratios, $\alpha_3 R_0^2/u_0$ and $\alpha_1 R_0^2/x_0$, are equal. This is peculiar to the case $\alpha = 2$ however, and does not hold for $\alpha = 3$. The con-

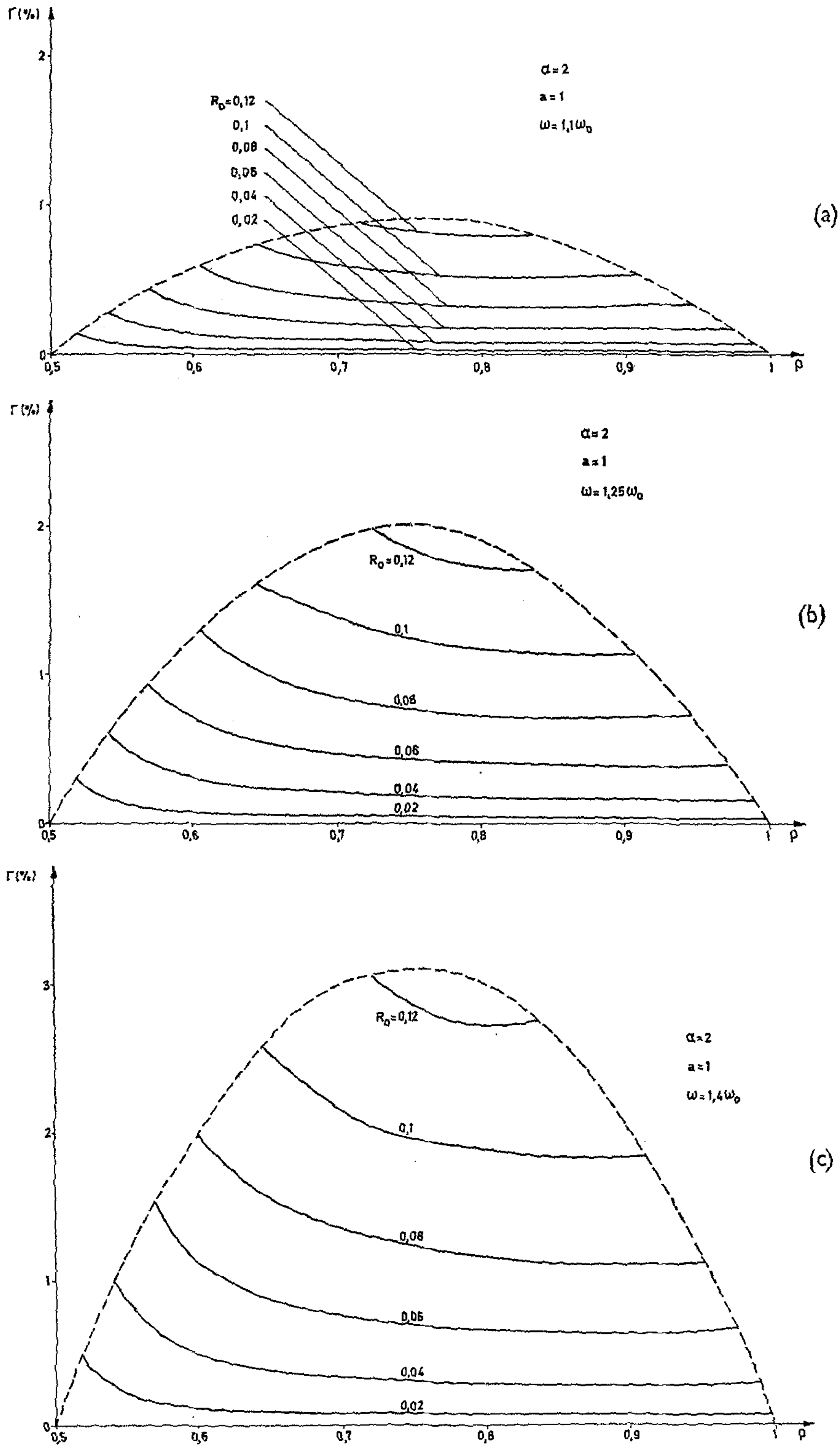


Figure 2. Per cent production gains Γ as a function of ρ, for varying oscillation amplitudes R_0 and frequencies ω, and for $\alpha = 2$ and $a = 1$. (a) $\omega = 1{,}1\omega_0$, (b) $\omega = 1{,}25\omega_0$, (c) $\omega = 1{,}4\omega_0$.

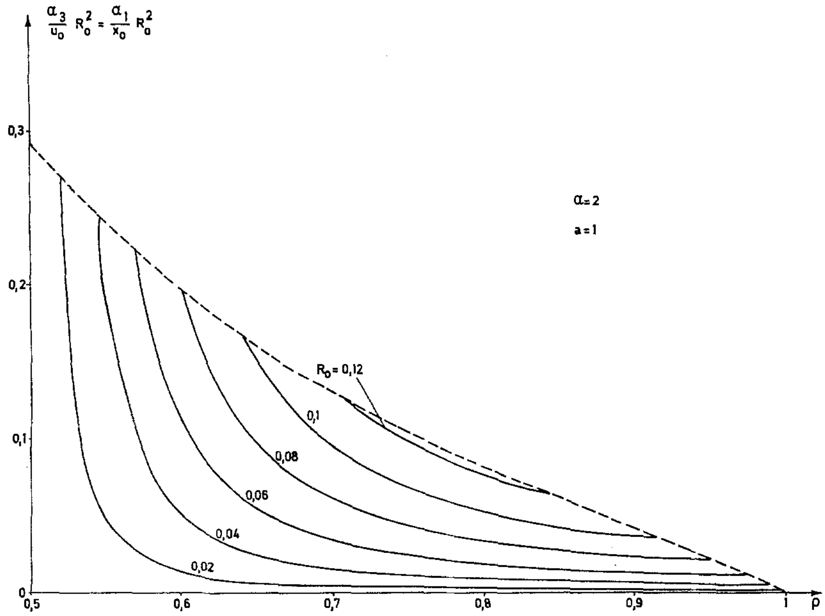


Figure 3. Constant terms in the control and state waveforms $\Delta u(t)$ and $\Delta x_1(t)$, relative to the optimal constant values u_0 and x_0, for $\alpha = 2$ and $a = 1$. Both ratios, $\alpha_3 R_0^2/u_0$ and $\alpha_1 R_0^2/x_0$ are equal.

stant terms are always positive, which means that in optimal periodic operation the average value of the control and state functions exceeds the optimal constant values. The bias becomes important for small values of ρ, but remains smaller than 30%. Again in this figure and in the subsequent ones, the dotted line denotes the physical bound, set by the condition $u(t) > 0$ for all t.

Figures 4–5 refer to the first and second harmonics of the control function $\Delta u(t)$. Figure 4a shows the amplitude of the first harmonic, relative to u_0. For a fixed R_0, the ratio increases as ρ approaches its upper and lower limits, causing the minimum of $u(t)$ to reach zero both at the higher and the lower sections of the range of ρ. The ratio may exceed 1 however, due to the positive constant term in $\Delta u(t)$, and due to the second harmonic which tends to flatten out the control waveform in the intervals where $\Delta u(t)$ is negative. This can be verified upon inspection of the phase angle diagrams in Figures 4b and 5b, which show that

$$\phi_2 + 2 \operatorname{arc\,tg}\left(\frac{\omega_0}{A}\right) \simeq \frac{3\pi}{2},$$

such that the second harmonic increases both the maximum and the minimum of the control function (see Figure 8 for some examples). Figure 4b also shows that the control and state oscillations are dephased by more than 90°, and that the dephasing approaches 180° as ρ approaches its lower limit.

The amplitude of the second harmonic, relative to u_0, is given in Figure 5a. The size of the second harmonic may amount to about 50% of the size of the fundamental harmonic, such that the control waveform is substantially nonsinusoidal.

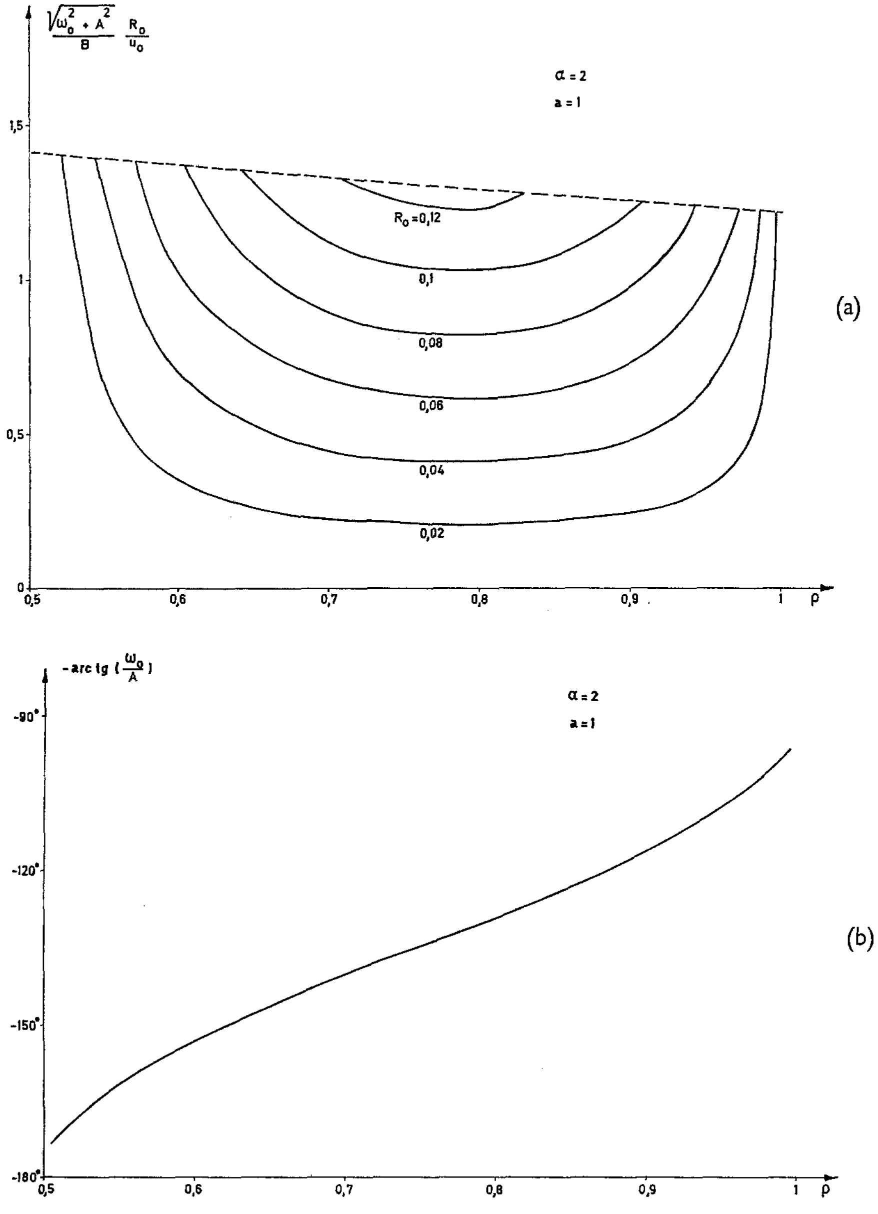


Figure 4. Control function $\Delta u(t)$: (a) ratio of fundamental harmonic amplitude $\sqrt{(\omega_0^2 + A^2)}R_0/B$ to optimal constant control u_0; (b) phase angle, $-\operatorname{arc\,tg}(\omega_0/A)$ of the control fundamental harmonic (case $\alpha = 2$, $a = 1$).

Figures 6 and 7 display the characteristics of the first and second harmonics of $\Delta x_1(t)$. Figures 6 and 7a show the relative amplitudes of the fundamental and second harmonics, R_0/x_0 and $\alpha_2 R_0^2/x_0$. The amplitude of the second harmonic has the order of magnitude of 10% to 15% of the amplitude of the fundamental harmonic. As a result, the state fluctuations are much closer to a pure sinusoid than the control fluctuations, and R_0 is close to the actual size of the state oscillation. As before, the dotted lines denote the boundary

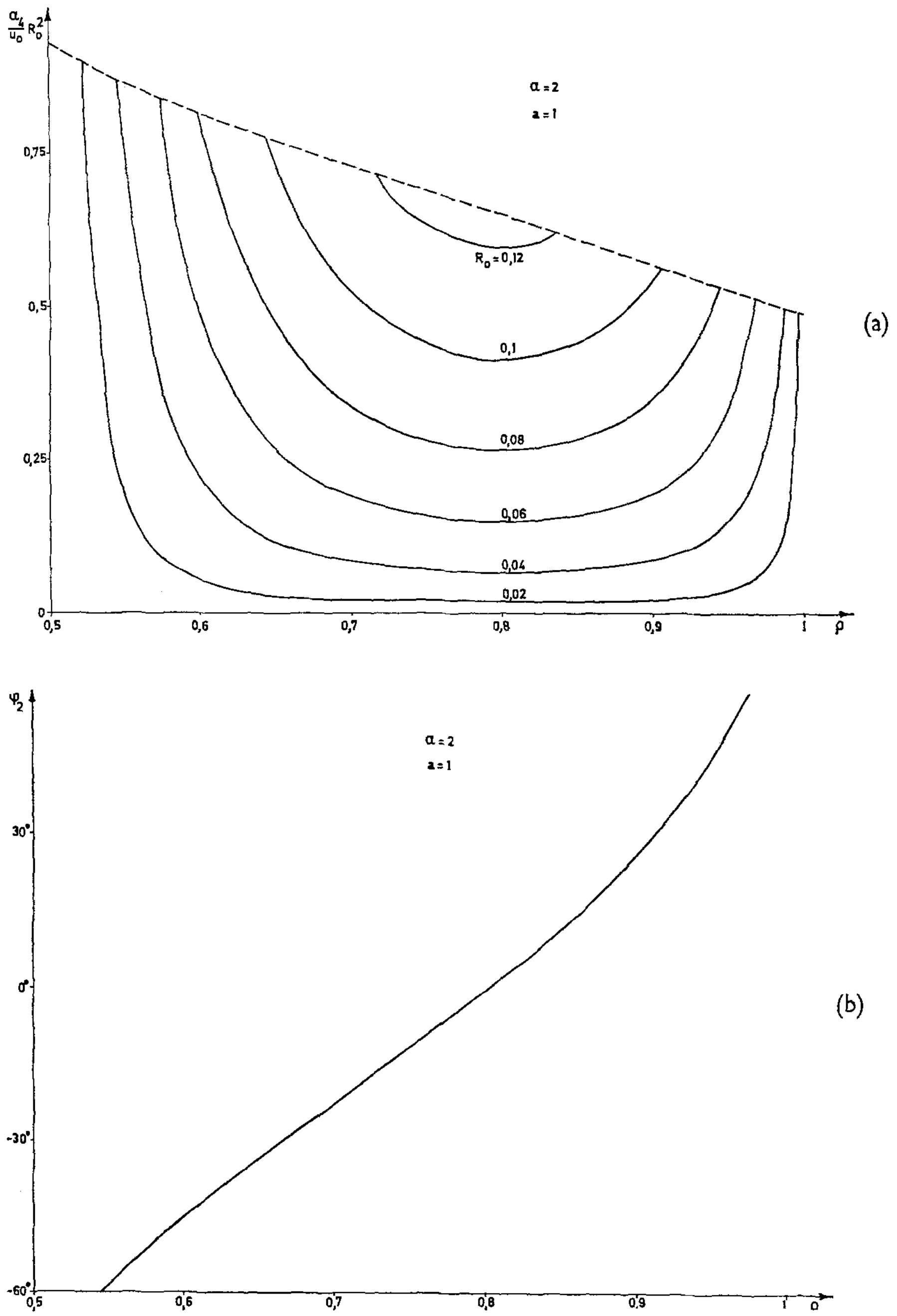


Figure 5. Control function $\Delta u(t)$: (a) ratio of second harmonic amplitude $\alpha_4 R_0^2$ to optimal constant control u_0; (b) phase angle ϕ_2 of second harmonic (case $\alpha = 2$, $a = 1$).

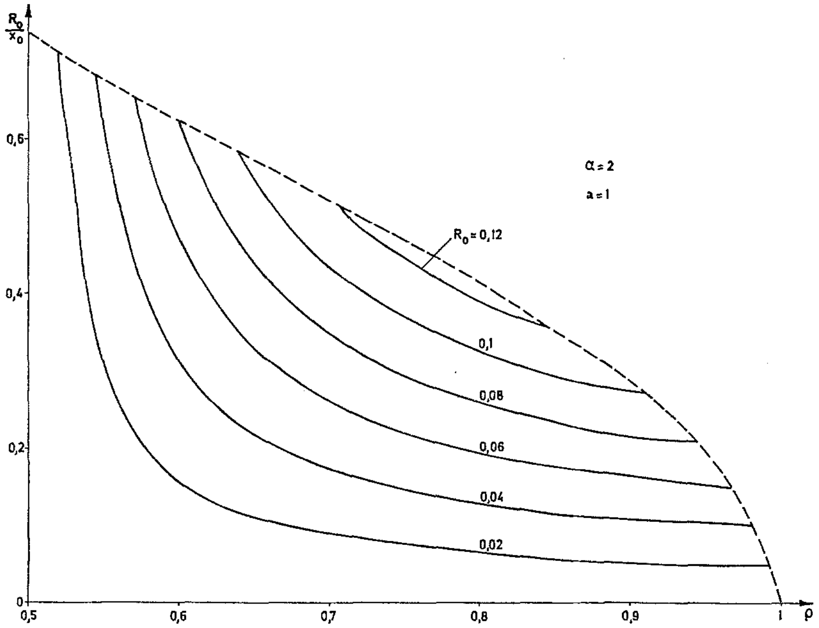


Figure 6. State function $\Delta x_1(t)$: ratio of fundamental harmonic amplitude R_0 to optimal constant state x_0 (case $\alpha = 2$, $a = 1$).

where the minimum value of the control function $u(t)$ becomes zero. At any point below this line, the sum of the relative amplitudes of the first and second harmonics of $\Delta x_1(t)$ is smaller than approximately 0,7. Hence the condition $x_1(t) > 0$ is certainly satisfied in this region. This shows that the present analysis, and the modes of operation resulting from it, are truly limited by the physical bounds on the control fluctuations, and not by the state fluctuations.

In Figure 8 the control and state waveforms have been computed as functions of time, for a given set of process parameters and for $R_0 = 0{,}04$ and $R_0 = 0{,}1$. For $R_0 = 0{,}04$ the constant terms in $\Delta u(t)$ and $\Delta x_1(t)$ are both very small, while the second harmonic of $\Delta x_1(t)$ is completely negligible. The state oscillation is approximately sinusoidal, while the control oscillation contains a second harmonic which increases both the maximum and the minimum of the waveform. The same effect appears for $R_0 = 0{,}1$, but the second harmonic is more important, and becomes discernible in the state oscillation as well. Also the constant terms in $\Delta u(t)$ and $\Delta x_1(t)$ have increased in size.

In the case where $\alpha = 3$, the results are completely analogous to the case $\alpha = 2$, except for numerical differences. For example, the curves yielding the relative production gains Γ as functions of ρ and R_0, for a given frequency ω, are quite similar in shape to those for $\alpha = 2$. Again, Γ increases with both increasing frequency and amplitude of oscillation. However, the numerical values of Γ are consistently about 50% larger than in the case $\alpha = 2$, and the interval for ρ, where production increases by cycling are possible, becomes $\{0{,}333 < \rho < 1\}$. Also the general characteristics of the control and state waveforms and the discussions related to them remain unaffected, except that now the relative value of the constant term in $\Delta u(t)$ is larger than the corresponding term in $\Delta x_1(t)$.

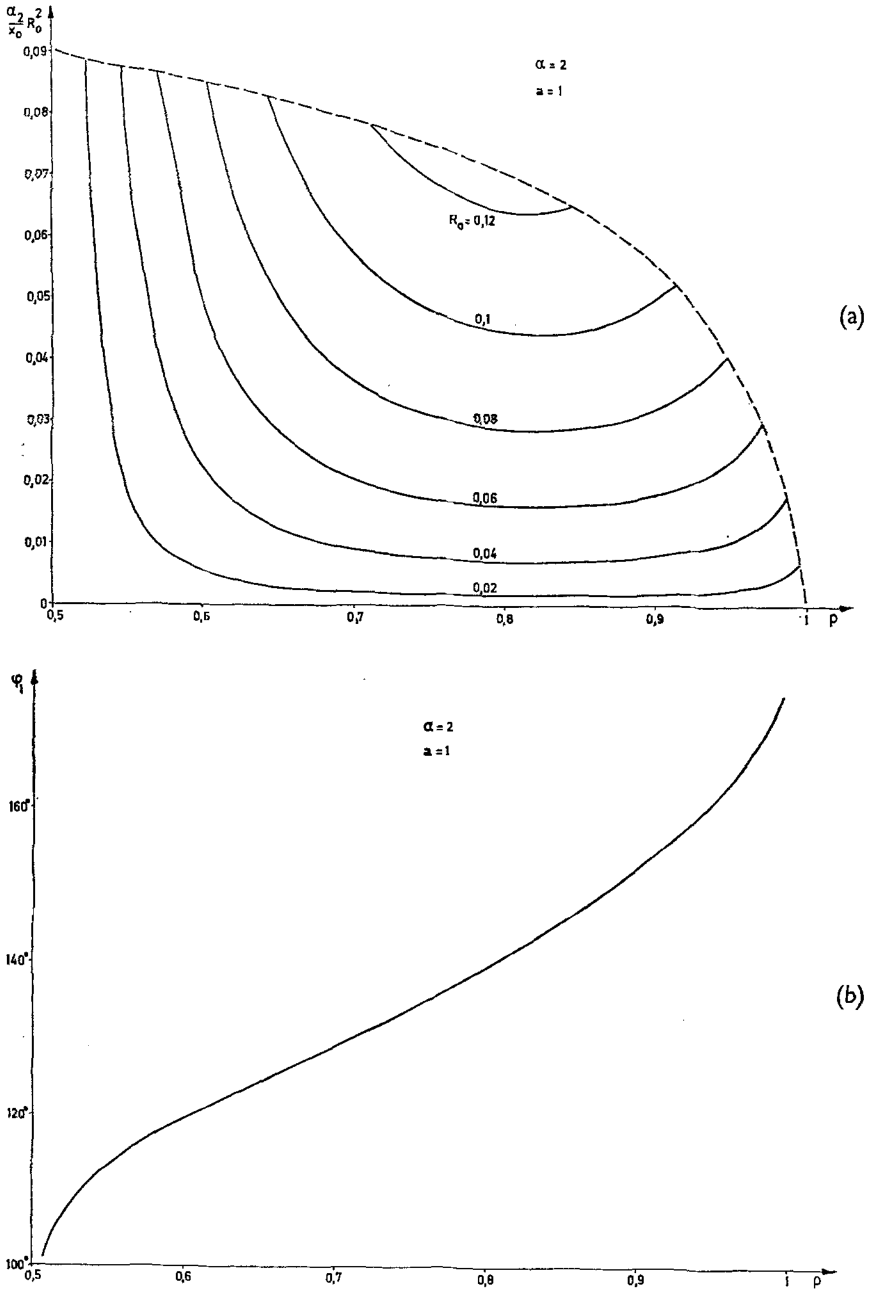
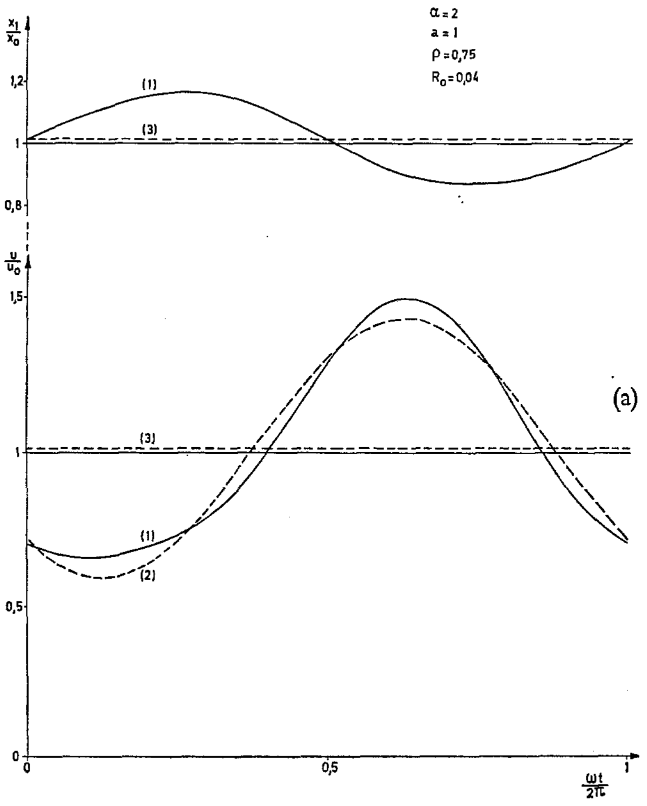
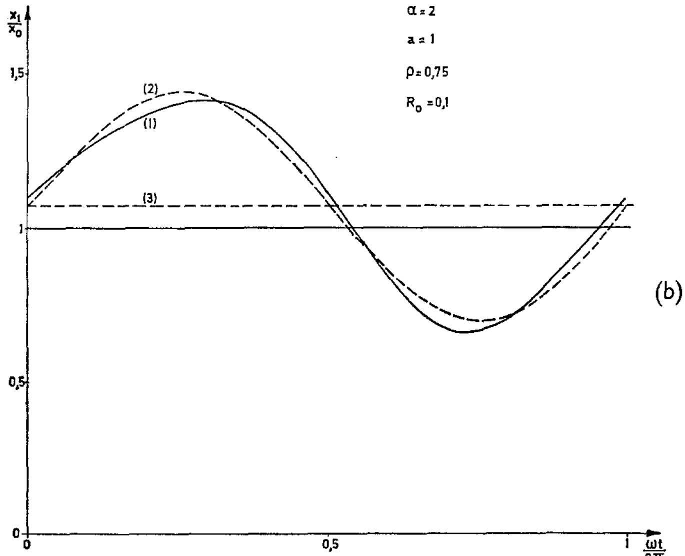


Figure 7. State function $\Delta x_1(t)$: (a) ratio of second harmonic amplitude $\alpha_2 R_0^2$ to optimal constant state x_0 (b) phase angle ϕ_1 of second harmonic (case $\alpha = 2$, $a = 1$).

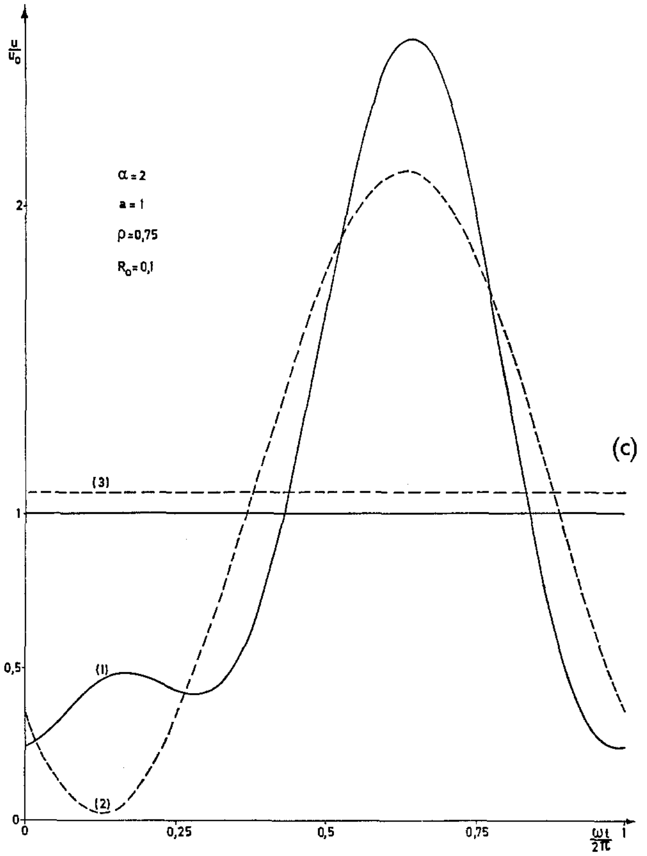


(a)



(b)

Figure 8. Time course of the control and state functions, relative to the optimal constant values, for $\alpha = 2$, $a = 1$ and $\rho = 0{,}75$, and for two different values of R_0. (a) state and control functions for $R_0 = 0{,}04$; (b) state function for $R_0 = 0{,}1$; (c) control function for $R_0 = 0{,}1$.
(1): waveforms up to the second harmonic; (2): waveforms up to the first harmonic; (3): the constant terms.



6. Conclusion

The optimal periodic operation has been investigated of a CSTR in which two parallel reactions take place, and which is controlled by reaction temperature. An approximate solution to the periodic optimization problem has been constructed, for small amplitude oscillations, and at frequencies slightly larger than the minimum frequency above which cycling may improve the optimal constant operation. The solution has been obtained using a perturbation technique, exploiting a simple mathematical connection that has been recognized between the π-criterion, and the necessary conditions for an optimal periodic control. The per cent production increases have been obtained as functions of the system parameters, and the frequencies and amplitudes of the oscillations that can be allowed to exist in the system. For given frequencies and given system parameters, the maximum attainable production gains in the analysed type of operation, are limited by the physical bounds on the control fluctuations. It has been shown that production gains increase with both frequency and amplitude of oscillation. The control and state waveforms have been studied up to the second harmonics. The state oscillations are close to a pure sinusoid, while the control functions contain an important second harmonic. The average value of the control and state functions exceeds the optimal constant values.

Several of these properties, for example the increase of production gains with both frequency and amplitude, are qualitatively well known from previous studies. The main merit and novelty of the present approach, is that it provides an analytical means of numerically computing the optimal periodic solution for an, albeit narrow, range of intermediate frequencies, and for small forcing amplitudes. Thus an estimate is produced of the maximum production gains that theoretically could be realized in periodic operation, using the considered oscillation frequencies and amplitudes. Also the time course and Fourier coefficients of the corresponding cyclic motions in the system may be analytically obtained. Such information may be useful to determine, under what conditions periodic operation of an industrial process might be successfully attempted, and even could be of some help in the design procedures for the controllers to be developed.

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