Higher-Order Corrections to the Pi Criterion Using Center Manifold Theory

Costas Kravaris*, Ioannis Dermitzakis, Scott Thompson
Department of Chemical Engineering, University of Patras, Patras, Greece

The frequency-dependent pi criterion of Bittanti et al. [7] is a very important tool that has been used extensively in applications, to predict potential performance improvement under periodic forcing in a nonlinear system. The pi criterion is local in nature and provides an approximate formula for the performance index under small-amplitude periodic forcing. Motivated by basic results from Center Manifold theory, the present work develops higher-order approximations, suitable for periodic forcing functions of larger amplitude. The proposed method is based on solving the Center Manifold partial differential equation via power series. The end result of the proposed approach is the approximate calculation of the performance index in the form of a truncated series expansion, which provides accurate results under larger amplitudes. The proposed method is applied to a continuous stirred tank reactor, where the yield of the desired product must be maximized.

Keywords: Optimal periodic control, nonlinear systems, center manifold theory, pi criterion.

1. Introduction

Center manifold theory has found many applications in problems of nonlinear dynamics [9], while at the same time, it is a powerful tool for solving output regulation problems for nonlinear systems [8]. The purpose of the present paper is to apply, for the first time, results from center manifold theory in the context of periodic control, where the average value of a nonlinear function of the states must be optimized.

Problems of periodic control are very important in the operation of chemical reactors, where the average yield or selectivity can be significantly improved if periodic forcing is used instead of constant-input operation. The first paper on periodic optimal control appeared in the chemical engineering literature in the late 60’s [14]; it used a variational approach to derive necessary conditions for optimality under periodic forcing. The work of Horn and Lin immediately caught the attention of many chemical reactor theorists, who showed that periodic forcing can potentially result in major improvements in yield and/or selectivity for many common chemical reaction systems ([2], [3]) see also review papers by Bailey [4] and Guardabassi et al. [12].

The next major contribution in periodic optimal control was the work by Bittanti et al. [7], who developed the so-called pi criterion from second-variation analysis of the corresponding optimal control problem (See also Bernstein & Gilbert [5] and Bernstein [6] for refinements in the theory of the pi criterion). The pi criterion enables to determine whether periodic operation can be advantageous over constant-input operation and, moreover, it provides a method to approximately calculate potential performance improvement/degradation under small-amplitude periodic forcing, based on a simple formula. During the last three decades, the pi criterion has been widely used in many application problems, as a predictive tool (e.g. [1], [16],

*Correspondence to: C. Kravaris, E-mail: kravaris@chemeng.upatras.gr
[17], [18], [19], [20], [21], [22]). At the same time, the limitations of the pi criterion became evident, in terms of its calculation accuracy being restricted to small amplitudes ([10], [13]). The present paper will propose a method to calculate higher-order corrections to the pi-criterion for a sinusoidal input function, which will increase its accuracy and make it applicable to higher amplitudes. In addition, it will develop a systematic framework for the approximate calculation of the performance index for a system under a general periodic input. Preliminary results for the case of sinusoidal inputs were reported in Kravaris et al. [15] and for the case of square-wave inputs in Dermitzakis and Kravaris [11].

The paper is organized as follows. After a brief necessary review of the pi criterion in Section 2, Section 3 will outline the application of Center Manifold theory for the calculation of the steady state response of a dynamic system under periodic forcing. The proposed approach will be developed in Section 4 and our main results will be specialized to sine-wave forcing in Section 5. Finally, Section 6 will illustrate the proposed approach and results in a chemical reactor application.

1.1. Problem formulation

Throughout this work we will consider nonlinear dynamic systems of the form

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

where $u \in \mathbb{R}$ is the system input, $x \in \mathbb{R}^n$ is the system state and $f : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ is a real analytic function.

It will be assumed that system (1) is driven by an input which is a periodic function of time and appropriate initial conditions, so that the system state is also a periodic function of time. Associated with (1), the following performance index will be considered:

$$J = \frac{1}{T} \int_0^T g(x(t), u(t)) dt$$

where $T$ is the period, $g : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ is a real analytic function, and the objective is to maximize $J$. The performance index $J$ is the average value of $g(x(t), u(t))$ over the time interval $[0, T]$. Alternatively, the performance index can be expressed in terms of the frequency $\omega = 2\pi / T$ as

$$J = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} g(x(t), u(t)) dt$$

2. Review of the Pi Criterion (Bittanti et al., 1973)

Defining $H(x, u, \lambda) = g(x, u) + \lambda^T f(x, u)$

$$A = \frac{\partial f}{\partial x}(x_0, u_0), \quad P = \frac{\partial^2 H}{\partial x^2}(x_0, u_0, \lambda_0)$$

$$B = \frac{\partial f}{\partial u}(x_0, u_0), \quad Q = \frac{\partial^2 H}{\partial u^2}(x_0, u_0, \lambda_0)$$

$$G(s) = (sI - A)^{-1} B, \quad R = \frac{\partial^2 H}{\partial u \partial^2}(x_0, u_0, \lambda_0)$$

where $(x_0, u_0)$ represents a reference equilibrium point of (1) and

$$\lambda_0 \frac{\pi}{\omega} = -\left[\frac{\partial g}{\partial x}(x_0, u_0)\right]^{-1} \left[\frac{\partial f}{\partial x}(x_0, u_0)\right]^{-1},$$

the pi criterion is given by

$$\pi(\omega) = [G(\omega)]^T PG(\omega) + QG(\omega) + [G(\omega)]^T Q^T + R \quad (3)$$

Bittanti et al (1973) have shown that there exists a periodic input $u(t)$ such that $J > g(x_0, u_0)$ if there exists a frequency $\omega$ such that $\pi(\omega) > 0$, and conversely, if there exists a periodic input $u(t)$ such that $J > g(x_0, u_0)$, then there exists a frequency $\omega$ such that $\pi(\omega) \geq 0$. Moreover, for a sine wave input with amplitude $M$ and frequency $\omega$, i.e. $u(t) = M \sin \omega t$, the performance index can be approximated by

$$J = g(x_0, u_0) + \pi(\omega) \frac{M^2}{4} + o(M^2), \text{ for small } M. \quad (4)$$

From the above approximate expression it is evident that, as long as $M$ is sufficiently small and $\pi(\omega) > 0$ for some $\omega$, $J$ will be larger than $g(x_0, u_0)$ and therefore periodic forcing will offer an improvement over constant-input operation.

Remark 1: In the original derivation of the pi criterion by Bittanti et al, it was assumed that $(x_0, u_0)$ is the optimal equilibrium point, i.e. that $g(x_0, u_0)$ is maximized at the equilibrium point $(x_0, u_0)$. In this case, $x_0, u_0$ and $\lambda_0$ are related via

$$\frac{\partial g}{\partial x}(x_0, u_0) + \lambda_0 \frac{\partial f}{\partial x}(x_0, u_0) = 0.$$

However, it was later shown (see [20] and references therein) that the results remain valid even when $(x_0, u_0)$ is not the optimal equilibrium point.

From (4), it is seen that $\pi(\omega)$ is the coefficient of the quadratic approximation of the performance index $J$ for a small-amplitude sinusoidal input. In the following sections, we will develop a method for computing higher-order terms, thus generating a series expansion of $J$, for a general class of periodic inputs.
3. Steady state response of a dynamic system under periodic forcing

One of the applications of Center Manifold theory is the calculation of the steady state response of a nonlinear dynamic system under periodic forcing [9]. The calculation is based on the Center Manifold of an extended system, which is computed by solving a system of singular partial differential equations. In this section, we will provide a brief necessary review of the calculation of the steady-state response to a periodic input, since it will play a key role in subsequent sections. The reader is referred to the monograph by Carr for the underlying theory of Center Manifolds, upon which the calculation is based.

Consider again the dynamic system (1) and, without loss of generality, assume that the equilibrium point \((x_0, u_0) = (0, 0)\) by appropriate translation of axes. When (1) is driven by the periodic function \(u = h(\sin \omega t, \cos \omega t)\) with \(h(0,0) = 0\), where \(h : \mathbb{R}^2 \to \mathbb{R}\) is a real analytic function, or, equivalently, by the output of the dynamic system

\[
\begin{align*}
\dot{z} &= \begin{bmatrix} 0 & \omega \\ -\omega & 0 \end{bmatrix} z, \quad z(0) = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\
\dot{u} &= h(z)
\end{align*}
\]

(5)

the response of \(x(t)\) can be computed via the unforced response of the extended system

\[
\begin{align*}
\dot{x} &= f(x, h(z)) \\
\dot{z} &= \begin{bmatrix} 0 & \omega \\ -\omega & 0 \end{bmatrix} z
\end{align*}
\]

(6)

Assuming that the system (1) \(\dot{x} = f(x,u)\) is hyperbolically stable around the origin, an invariant manifold \(x = S(z)\) of the extended system (6) will be Center Manifold of (6) and the mapping \(S\) will satisfy the Center Manifold Equation (CME):

\[
\frac{\partial S(z)}{\partial z} \begin{bmatrix} 0 & \omega \\ -\omega & 0 \end{bmatrix} z = f(S(z), h(z)) \quad \text{or equivalently}
\]

\[
\omega \left( z_2 \frac{\partial S}{\partial z_1}(z_1, z_2) - z_1 \frac{\partial S}{\partial z_2}(z_1, z_2) \right) = f(S(z_1, z_2), h(z_1, z_2))
\]

(7)

and the initial condition \(S(0) = 0\).

Two very important properties of Center Manifolds [8], [9], will need to be reviewed at this point, as they apply to the particular system (6) under consideration. The first result establishes that the solutions of (6) asymptotically approach the Center Manifold, whereas the second result enables the approximation of the Center Manifold.

Result 1 – Attractivity of the Center Manifold: Suppose that all the eigenvalues of \(\frac{\partial S}{\partial z}(0,0)\) have negative real parts and \(S(z)\) satisfies the CME (7) with \(S(0) = 0\). Then there exist constants \(K > 0, \beta > 0\) such that, for initial conditions \((x(0), z(0))\) near the origin, the solution \((x(t), z(t))\) of (6) satisfies

\[
\|x(t) - S(z(t))\| \leq Ke^{-\beta t} \|x(0) - S(z(0))\| \quad \text{for all } t \geq 0.
\]

The above result establishes that \(x(t)\) asymptotically approaches \(S(z(t))\) in the limit as \(t \to \infty\); this is the so-called “steady-state response” of system (1) under the periodic input \(u(t)\) generated by system (5). Hence, the steady-state response of \(x(t)\) is given by

\[
x(t) = S(\sin \omega t, \cos \omega t)
\]

(8)

Result 2 – Approximation of the Center Manifold: Suppose that \(S(z)\) satisfies the CME (7) with \(S(0) = 0\). Also, let \(\phi\) be a \(C^1\) mapping from a neighborhood of the origin of \(\mathbb{R}^2\) into \(\mathbb{R}^n\), such that \(\phi(0) = 0\) and

\[
\omega \left( z_2 \frac{\partial \phi}{\partial z_1}(z_1, z_2) - z_1 \frac{\partial \phi}{\partial z_2}(z_1, z_2) \right) = f(\phi(z_1, z_2), h(z_1, z_2))
\]

\[= O(\|z\|^q) \quad \text{as } z \to 0 \quad \text{with } q > 1.
\]

Then \(\|S(z) - \phi(z)\| = O(\|z\|^q) \quad \text{as } z \to 0\).

The above result establishes that the Center Manifold can be approximated to any degree of accuracy if the CME (7) can be approximately satisfied at the same level of accuracy. For example, using a power series approach, the CME can be satisfied up to any desirable order \(q\). Then, as long as system (6) possesses an analytic Center Manifold \(x = S(z)\), the power series will converge to it.

3.1. The input function

In the above problem formulation, the periodic function that drives the dynamic system is assumed to be a function of sines and cosines. This includes sine wave functions and also, all periodic functions that can be adequately approximated by a truncated Fourier series.

The sine wave of amplitude \(M\) and frequency \(\omega\) is, of course, the simplest example:

\[
u = M \sin \omega t
\]

which corresponds to

\[
h(z) = M \cdot z_1.
\]

(9)
Another commonly used periodic function is a square wave of amplitude $M$ and period $\frac{2\pi}{\omega}$, whose Fourier series expansion is $M = \frac{4}{\pi} \left( \sin \omega t + \frac{\sin 3\omega t}{3} + \frac{\sin 5\omega t}{5} + \ldots \right)$. This can be appropriately truncated to:

$$u = M \frac{4}{\pi} \left( \sin \omega t + \frac{\sin 3\omega t}{3} + \ldots + \frac{\sin p\omega t}{p} \right)$$

for some $p = \text{odd number}$. Using the multiple-angle formulas for sines, the above periodic function can be expressed as a polynomial of odd powers of $\sin \omega t$, therefore the corresponding function $h(z)$ is a polynomial of odd powers of $z_1$. In particular,

$$h(z) = M \frac{4}{\pi} \sum_{k=0}^{p-1} (-1)^{p-k} k^{p-2k-1} \frac{p-k}{p-2k} \cdot z_1^{p-2k} \quad (10)$$

In general, any square-integrable zero-mean periodic function of period $\frac{2\pi}{\omega}$ can be expanded in Fourier series of the form

$$u = \sum_{n=1}^{\infty} (a_n \sin n\omega t + b_n \cos n\omega t)$$

Truncating the Fourier series and using the multiple-angle formulas for sines and cosines, the above periodic function can be expressed as a polynomial of powers of $\sin \omega t$ and $\cos \omega t$, hence the function $h(z)$ will be a polynomial of $z_1$ and $z_2$.

**Remark 2:** There are many alternative approaches for approximating a non-sinusoidal periodic function by a function of sinusoids. For example, a square wave of amplitude $M$ and period $\frac{2\pi}{\omega}$ can be alternatively approximated as $M \tanh(k \sin(\omega t))$, for sufficiently large $k$ (of the order of 10 or higher). Truncated Fourier series is the most popular general approach, in view of its practical advantages.

**4. Proposed Approach**

The results of the previous section enable the calculation of the steady-state response $x(t)$ of $\dot{x} = f(x, u)$ via equation (8), with the function $S$ being obtained from a power-series solution of equation (7). The result for the steady-state response can be substituted in the integrand of the expression for the performance index

$$J = \frac{\omega}{2\pi} \int \frac{2\pi}{\omega} g(x(t), u(t)) dt$$

and, in this way, the performance index can be calculated. Thus:

$$J = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} g(S(\sin \omega t, \cos \omega t), h(\sin \omega t, \cos \omega t)) dt$$

where $S : \mathbb{R}^2 \rightarrow \mathbb{R}^n$ is the solution of the Center Mainfold Equation (CME)

$$\omega \left( z_2 \frac{\partial S}{\partial z_1} (z_1, z_2) - z_1 \frac{\partial S}{\partial z_2} (z_1, z_2) \right) = f(S(z_1, z_2), h(z_1, z_2))$$

with initial condition $S(0) = 0$.

The proposed approach involves the following steps:

**Step 1:** Series solution of the CME

**Step 2:** Substitution of the result for $S(z)$ into the expression for $J$ and calculation of the integral in the form of series.

The end result from the proposed approach will be an expression for $J$ as a function of the amplitude $M$ and the frequency $\omega$ in the form of a series expansion.

Also, it will be shown that, in the case of a sine wave input, the quadratic approximation of the solution of the PDE and of the integrand in the performance index will give rise to the well known pi criterion.

**4.1. Power series solution of the CME**

Consider again the Center Mainfold Equation (7). To be able to derive conditions that determine the Taylor coefficients of the unknown solution, it will be convenient to use tensorial notation for the partial derivatives.

Defining

$$f_{\mu}^i = \frac{\partial f}{\partial x_j} (0, 0), \quad f_{\mu}^i = \frac{\partial f}{\partial u} (0, 0), \quad f_{\mu}^{ij} = \frac{\partial^2 f}{\partial x_j \partial x_j} (0, 0), \quad f_{\mu}^{ij} = \frac{\partial^2 f}{\partial x_j \partial u} (0, 0), \quad \text{etc.}$$

and similar notation for the partial derivatives of $S(z)$ and $h(z)$, and using the standard summation convention, the matching of the coefficients of like terms in the Taylor series expansion of the PDE yields the following conditions:

**First-order terms:**

$$-\omega S_{\mu}^2 = f_{\mu}^i \cdot z_1^1 + f_{\mu}^u^1 h^1$$

$$\omega S_{\mu}^1 = f_{\mu}^i \cdot z_1^2 + f_{\mu}^u^2 h^2$$
Second-order terms:
\[ -2\omega S_{\mu}^{12} = f^{ij}_{\mu} S_{j1}^{11} + f_{\mu}^u h_{11}^1 + f^{ij}_{\mu}^j S_{j1}^{1} S_{j2}^{1} \\
+ 2f^{ij}_{\mu}^j h_{11}^1 S_{j1}^{1} + f_{\mu}^{au} (h^1)^2 \]
\[ \omega (S_{\mu}^{11} - S_{\mu}^{22}) = f^{ij}_{\mu} S_{j1}^{12} + f_{\mu}^u h_{12}^1 + f^{ij}_{\mu}^j S_{j1}^{1} S_{j2}^{1} \\
+ f_{\mu}^{ua} (h^1)^2 S_{j1}^{1} + f_{\mu}^{au} (h^1)^2 \]
\[ 2\omega S_{\mu}^{12} = f^{ij}_{\mu} S_{j1}^{22} + f_{\mu}^u h_{22}^1 + f^{ij}_{\mu}^j S_{j1}^{2} S_{j2}^{1} + 2f_{\mu}^{au} (h^2)^2 \]
Third-order terms:
\[ -3\omega S_{\mu}^{111} = f^{ij}_{\mu} S_{j1}^{111} + f_{\mu}^u h_{111}^1 + 3f^{ij}_{\mu}^j S_{j1}^{1} S_{j1}^{1} S_{j1}^{1} \\
+ 3f_{\mu}^{au} h_{111}^1 + f^{ij}_{\mu}^j S_{j1}^{1} S_{j1}^{1} S_{j1}^{1} \\
+ 3f_{\mu}^{au} h_{111}^1 + f^{ij}_{\mu}^j h_{111}^1 S_{j1}^{1} + 3f_{\mu}^{au} (h^1)^2 S_{j1}^{1} + f_{\mu}^{au} (h^1)^3 \]
\[ \omega (S_{\mu}^{11} - 2S_{\mu}^{12}) = f^{ij}_{\mu} S_{j1}^{11} + f_{\mu}^u h_{11}^2 + f^{ij}_{\mu}^j S_{j1}^{1} S_{j1}^{1} S_{j1}^{1} \\
+ f_{\mu}^{ua} (h^2)^2 S_{j1}^{1} + f_{\mu}^{au} (h^2)^2 \]
\[ \omega (2S_{\mu}^{12} - S_{\mu}^{222}) = f^{ij}_{\mu} S_{j1}^{122} + f_{\mu}^u h_{12}^2 \\
+ f^{ij}_{\mu}^j (S_{j1}^{22} + 2S_{j1}^{1} S_{j1}^{1}) \\
+ f_{\mu}^{ua} (h^2)^2 S_{j1}^{1} + f_{\mu}^{au} (h^2)^2 \]
\[ 3\omega S_{\mu}^{111} = f^{ij}_{\mu} S_{j1}^{111} + f_{\mu}^u h_{11}^2 + f^{ij}_{\mu}^j S_{j1}^{1} S_{j1}^{1} S_{j1}^{1} \\
+ f_{\mu}^{ua} (h^2)^2 S_{j1}^{1} + 3f_{\mu}^{au} h_{11}^2 + 3f^{ij}_{\mu}^j S_{j1}^{1} S_{j1}^{1} S_{j1}^{1} \\
+ f_{\mu}^{au} (h^2)^2 \]
eq etc.

(i) The condition arising from the matching of coefficients of the terms \( z_1 z_2 \cdots z_{i_N} \) can be written in general as
\[ L_{\mu}^{i_1 \cdots i_N} = R_{\mu}^{i_1 \cdots i_N}, \quad \mu = 1, \ldots, n, \quad i_1, \ldots, i_N = 1, 2 \]
where \( L(z) = \omega(z_1 \partial z_2 (z) - z_1 \partial z_2 (z)) \) is the left-hand side of the PDE and \( R(z) = f(S(z), h(z)) \) is the right-hand side.
(ii) It is not difficult to prove by induction that
\[ R_{\mu}^{i_1 \cdots i_N} = f^{ij}_{\mu} S_{j1}^{i_1 \cdots i_N} + \left( \text{Polynomial of } S_{j1}^{i_1 \cdots i_N} \right) \]
(j = 1, \ldots, n, \ i_1, \ldots, i_k = 1, 2, \ k = 1, \ldots, N - 1)
(with the index \( j_1 \) running from 1 through \( n \) in the summation in the first term).
(iii) It is not difficult to derive a general expression for the Taylor coefficients of the left-hand side. In particular, defining
\[ S_{\mu}^{i_1 \cdots i_k} = S_{\mu}^{1 \cdots 1 i_2 \cdots i_k} = \delta^{i_1 + i_2}_0 S_{\mu}^{i_2 i_2 \cdots i_k}, \quad i_1, i_2, \cdots, i_k \in N \]
and \( L_{\mu}^{i_1 \cdots i_k} = L_{\mu}^{1 \cdots 1 i_2 \cdots i_k} = \delta^{i_1 + i_2}_0 L_{\mu}^{i_2 i_2 \cdots i_k}, \) it is easy to see that they are related through the following relations:
\[ L_{\mu}^{i_1 \cdots i_k} = \omega(-i_1 \cdot S_{\mu}^{i_1, i_1 + 1}) \]
\[ L_{\mu}^{i_1 \cdots i_k} = \omega((i_1 \cdot S_{\mu}^{i_1 + 1, i_1 - 1} - i_1 \cdot S_{\mu}^{i_1 - 1, i_1 + 1}) \cdot i_2, i_3, \cdots, i_k \in N \]
\[ L_{\mu}^{i_1 \cdots i_k} = \omega \cdot i_1 \cdot S_{\mu}^{i_1, i_1 - 1} \]

hence every Taylor coefficient of the left-hand side is a linear combination of Taylor coefficients of \( S(z) \) of order \( N \) depending also on the coefficients of order \( (N - 1) \) and lower.
(iv) The conclusion from the above is that the conditions arising from the matching of \( N \)-th order terms of the PDE are linear equations with respect to the Taylor coefficients of \( S(z) \) of order \( N \), depending also on the coefficients of order \( (N - 1) \) and lower.

Therefore, to obtain the coefficients of the power series of \( S(z) \) up to a given truncation order \( N \), one must first solve 2n linear equations for the 2n unknowns in \( S^1 \) and \( S^2 \). Then, given the result for \( S^1 \) and \( S^2 \), one must solve 3n linear equations for the 3n unknowns in \( S^{11}, S^{22} \) and \( S^{12} \). Then, given the result for \( S^1, S^2, S^{11}, S^{22} \) and \( S^{12} \), one must solve 4n linear equations for the 4n unknowns in \( S^{111}, S^{112}, S^{122}, S^{222} \). etc. At the \( N \)-th step of this procedure, given the Taylor coefficients of \( S(z_1, z_2) \) up to \( (N - 1) \)-th order, one must solve \( (N + 1) \)-th linear equations to determine the \( N \)-th order Taylor coefficients of \( S(z_1, z_2) \). All these calculations can be carried out easily, with the aid of a symbolic software package, like Maple.
4.2. Approximate expansion of the performance index

Once the function $S(z_1, z_2)$ has been computed in the form of truncated power series, the same must be done for the function

$$\Psi(z_1, z_2) = g(S(z_1, z_2), h(z_1, z_2))$$

which appears in the integrand in the expression for the performance index:

$$J = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} \Psi(\sin \omega t, \cos \omega t) dt$$

followed by term-by-term integration of the power series. The result will be an approximate expansion for $J$, depending on the amplitude $M$ and the frequency $\omega_0$.

Indeed, expanding

$$\Psi(z_1, z_2) = g(0, 0) + \Psi^1 z_1 + \Psi^2 z_2 + \sum_{n=1}^{\infty} a_n (z_1 z_2)^n$$

etc., and using the formula

$$\omega \int_0^{2\pi/\omega} \frac{\sin^{N-m} \omega t \cos^m \omega t}{(N-m)!m!} dt = \begin{cases} 1 & \text{if both } N, m \text{ are even} \\ 0 & \text{otherwise} \end{cases}$$

the result is

$$J = g(0, 0) + \frac{1}{2} \left( \Psi^1 + \Psi^2 \right) + \frac{1}{2^4(2^3)} \left( \Psi^{11} + 2\Psi^{12} + \Psi^{22} \right) + \frac{1}{2^6(3^5)} \left( \Psi^{111} + 3\Psi^{112} + 3\Psi^{122} + \Psi^{222} \right) + \cdots$$

A second-order approximation of $S(z)$ leads to the approximation of the performance index

$$J^{2nd} = g(0, 0) + \frac{1}{2} \left( \Psi^1 + \Psi^2 \right) + g^u (h^1 + h^2) + g^{iij}(S^1_{ij} + S^2_{ij}) + 2g^{iij}(h^1 S^1_{ij} + h^2 S^2_{ij}) + g^{uu} (h^1)^2 + (h^2)^2$$

a fourth-order approximation of $S(z)$ leads to the approximation of the performance index

$$J^{4th} = g(0, 0) + \frac{1}{2} \left( \Psi^1 + \Psi^2 \right) + \frac{1}{2^4(2^3)} \left( \Psi^{11} + 2\Psi^{12} + \Psi^{22} \right)$$

and so on. In general, $J^{Nth}$ ($N$ = even), will depend upon the Taylor coefficients of the $N$-th order truncation of $S(z)$.

5. Series expansion of the performance index for sine wave input

In the present section, it will be shown that in the case of a sine wave input,

$$h(z) = M \cdot z_1$$

the foregoing series expansion becomes exactly a power series expansion of $J$ in the amplitude $M$, with the second-order approximation being exactly (4), i.e. giving rise to the pi criterion.
At first, one must establish the following important property of the solution \( S(z) \) of the CME in the case \( h(z) = M \cdot z_1 \):

**Proposition 1:** Let \( s(z) = [S(z)]_{M=1} \), i.e., \( S(z) \) is the solution of

\[
\omega \left( z_2 \frac{\partial s}{\partial z_1} (z_1, z_2) - z_1 \frac{\partial s}{\partial z_2} (z_1, z_2) \right) = f(s(z_1, z_2), z_1)
\]

\( s(0) = 0 \)

Then

\[
S(z_1, z_2) = s(Mz_1, Mz_2).
\]

**Proof:** Applying (13) with \( z_1 \to Mz_1 \) and \( z_2 \to Mz_2 \) results in

\[
\omega \left( Mz_2 \frac{\partial s}{\partial z_1} (Mz_1, Mz_2) - Mz_1 \frac{\partial s}{\partial z_2} (Mz_1, Mz_2) \right)
= f(s(Mz_1, Mz_2), Mz_1).
\]

Defining \( S(z_1, z_2) = s(Mz_1, Mz_2) \), it follows

\[
\frac{\partial S}{\partial z_1} (z_1, z_2) = M \frac{\partial s}{\partial z_1} (Mz_1, Mz_2)
\]

and

\[
\frac{\partial S}{\partial z_2} (z_1, z_2) = M \frac{\partial s}{\partial z_2} (Mz_1, Mz_2).
\]

Therefore

\[
\omega \left( z_2 \frac{\partial S}{\partial z_1} (z_1, z_2) - z_1 \frac{\partial S}{\partial z_2} (z_1, z_2) \right) = f(S(z_1, z_2), Mz_1)
\]

Hence \( S(z_1, z_2) \) is the solution of the CME for \( h(z) = Mz_1 \).

**5.1. Power series expansion of the performance index with respect to the amplitude M**

An immediate consequence of the foregoing proposition is that for \( h(z) = Mz_1 \),

\[
S^{\mu_1, \cdots, \mu_n}_{i_1, \cdots, i_N} = M^n \cdot s^{\mu_1, \cdots, \mu_n}_{i_1, \cdots, i_N}, \quad \mu = 1, \cdots, n, \quad i_1, \cdots, i_N = 1, 2
\]

(14)

i.e. the \( N \)-th order coefficients of the power series expansion of \( S(z) \) are proportional to \( M^n \).

Moreover, defining \( \psi(z) = [\Psi(z)]_{M=1} = g(s(z_1, z_2), z_1) \), it follows that \( \Psi(z_1, z_2) = \psi(Mz_1, Mz_2) \) and therefore

\[
\psi^{\mu_1, \cdots, \mu_n}_{i_1, \cdots, i_N} = M^n \cdot \psi^{\mu_1, \cdots, \mu_n}_{i_1, \cdots, i_N}, \quad \mu = 1, \cdots, n, \quad i_1, \cdots, i_N = 1, 2
\]

Thus, the expansion (12) of the performance index takes the form

\[
J = g(0, 0) + (\psi^{11} + \psi^{22}) M^2 + (\psi^{11} + 2\psi^{12} + \psi^{22}) M^4
+ (\psi^{1111} + 3\psi^{1112} + 3\psi^{1212} + \psi^{2222}) M^6
+ (\psi^{111111} + 4\psi^{111112} + 6\psi^{111222} + 4\psi^{112222} + \psi^{222222}) M^8
+ \cdots
\]

(15)

Setting

\[
\pi(\omega) = \psi^{11} + \psi^{22} = \rho(\omega) + \sigma(\omega) \omega^2 + \tau(\omega) \omega^4
\]

(16)

\[
\rho(\omega) = \psi^{1111} + 2\psi^{1112} + \psi^{2222}
\]

\[
\sigma(\omega) = \psi^{111111} + 3\psi^{111112} + 3\psi^{111222} + \psi^{222222}
\]

\[
\tau(\omega) = \psi^{11111111} + 4\psi^{11111112} + 6\psi^{11111222} + 4\psi^{11112222} + \psi^{22222222}
\]

\[
\cdots \cdots \cdots
\]

the performance index \( J \) can be expressed in the form

\[
J = J_0 + \pi(\omega) \frac{M^2}{2^2} + \rho(\omega) \frac{M^4}{2^4(2!)^2} + \sigma(\omega) \frac{M^6}{2^6(3!)^2}
+ \tau(\omega) \frac{M^8}{2^8(4!)^2} + \cdots
\]

(17)

with \( \pi(\omega) \) being determined by the 2nd-order approximation of \( s(z) \),
\( \rho(\omega) \) being determined by the 4th-order approximation of \( s(z) \),
\( \sigma(\omega) \) being determined by the 6th-order approximation of \( s(z) \),

**Remark 3:** In the case of an approximated square wave input (10) with \( p > 1 \), (14) no longer holds. Because in this case the function \( h(z) \) equals \( M \) times a polynomial of odd powers of \( z_1 \) (see (10)), it turns out that the \( N \)-th order coefficients of the power series expansion of \( S(z) \) are linear combinations of

\[
M^n, M^{N-2}, \cdots, M^{N-2y}
\]
where \( \gamma = \left( \frac{1}{2} (N - 1) - \left\lfloor \frac{N - 1}{2} \right\rfloor \right) \) with \( \lfloor \cdot \rfloor \) denoting the integer part of a real number.

Note that for \( N = kp, k \in \mathbb{N} \), the lowest power of \( M \) is \( N - 2 \gamma = k \), whereas for \( N > kp, k \in \mathbb{N} \), the lowest power is \( N - 2 \gamma > k \). Therefore, for every \( k \in \mathbb{N} \), terms proportional to \( M^k \) arise in the Taylor coefficients of \( S(z) \) of order up to \( kp \).

With these observations in mind, it follows that for an approximate square wave input, the expansion (12) of the performance index can still be rearranged in the form (17), however with \( \pi(\omega) \) being determined by the \((2p)\)th – order approximation of the center manifold, \( \rho(\omega) \) being determined by the \((4p)\)th – order approximation of the center manifold, \( \sigma(\omega) \) being determined by the \((6p)\)th – order approximation of the center manifold, etc.

In general, for a periodic input function with \( h(z) \) equal \( M \) times a polynomial of \( z_1 \) and \( z_2 \), it is possible to expand the performance index as a power series of the amplitude, with frequency-dependent coefficients:

\[
J(\omega, M) = \sum_{\ell} c_\ell(\omega) M^\ell
\]

However, it will not necessarily involve only even powers of \( M \) and the coefficients \( c_\ell(\omega) \) will in general depend on approximations of the center manifold of order larger than \( \ell \).

5.2. Quadratic approximation gives rise to the pi criterion

When the foregoing expansion (17) for the performance index is truncated after the quadratic term in \( M \), an expression of the form of equation (4) is obtained. We will now show that \( \pi(\omega) \) given by equation (16) is exactly the pi criterion of Bittanti et al. [7].

At first, observe that the expression (16) for \( \pi(\omega) \) depends on \( s^1, s^2 \) and the sum \((s^1)^2 + (s^2)^2\). The latter can be obtained easily by adding the first and the third equation of the recursion relations for the second-order terms of §4.1, and substituting \( h(z) = z_1^2 \):

\[
0 = f_{ij}^{(1)} (s^1_j + s^1_j) + f_{i}^{(2)} (s^1_j + s^2_j) + 2 f_{i}^{(1)} s^1_j + f_{i}^{(2)}
\]

Setting \( V = \left[ \delta(0,0) \right]^{-1} \), we have \( V_v f_{i}^{(1)} = \delta_v^i \), \( v = 1, \ldots, n \), and therefore the \( v\)-th component of \((s^1)^2 + (s^2)^2\) can be expressed as follows:

\[
s^1_v + s^2_v = -V_v f_{i}^{(2)} (s^1_j + s^2_j) + 2 f_{i}^{(1)} s^1_j + f_{i}^{(2)}
\]

Substituting the above into the expression (16) for \( \pi(\omega) \), we obtain

\[
\pi(\omega) = \left( s^1 f_{i}^{(2)} + s^2 f_{i}^{(1)} (s^1_j + s^2_j) \right) + 2 (s^1 f_{i}^{(1)} s^1_j + f_{i}^{(2)}
\]

where \( \lambda_\mu = -g \), \( V_\mu, \mu = 1, \ldots, n \)

In the notation of Section 2, the above can be written as follows:

\[
\pi(\omega) = s^T P s^1 + s^T P s^2 + 2 Q s^1 + R
\]

and because \( P \) is a symmetric matrix, this can be written equivalently as

\[
\pi(\omega) = (s^1 - i s^2)^T P (s^1 + i s^2)
\]

But from the first-order conditions,

\[
s^1 = -A(2 + \omega^2 I) \quad B = Re \{ i o i - A \}^{-1} B \quad s^2 = -\omega (2 + \omega^2 I) \quad B = Im \{ i o i - A \}^{-1} B,
\]

where \( A = \frac{\gamma}{\eta}(0,0), B = \frac{\gamma}{\eta}(0,0) \), and therefore

\[
s^1 = i s^2 \quad (\omega o i - A)^{-1} B \quad s^1 = -i s^2 \quad (\omega o i - A)^{-1} B
\]

and so we conclude

\[
\pi(\omega) = \left( (\omega o i - A)^{-1} B \right) P (\omega o i - A)^{-1} B
\]

This is identical to the expression (3) of the pi criterion of Bittanti et al. [7].

6. Application to a chemical reactor

Consider a continuous stirred tank reactor (CSTR), where the following parallel reactions take place:

\[2A \rightarrow B \quad A \rightarrow C\]

Species A is the reactant, B is the desired product, and C is an undesired by-product. This reaction system was first studied by Horn & Lin [14], and later by Sterman & Ydstie [20] in the context of the pi criterion. It was found that, under certain conditions, the yield of the desired product B can be significantly improved if the reaction temperature is varied periodically with high frequency. In the present section, we will apply the theoretical results of the previous sections to this reaction system.

The dynamic model for the CSTR involves two component mass balances and has the following form (14):

\[
\frac{dx_1}{dt} = -ux_1^2 - \beta u^2 x_1 - x_1 + 1
\]

\[
\frac{dx_2}{dt} = ux_1 - x_2
\]
The system states $x_1$ and $x_2$ represent dimensionless concentrations of the reactant and the desired product respectively, whereas the input $u$ is a dimensionless nonlinear transformation of the reaction temperature. The objective is to maximize the average value of the concentration $x_2$ of the desired product.

The CSTR system dynamics is of the form of (1) with $f(x,u) = \left[-ux_1^2 - \beta ux_1 - x_1 + 1\right]$ and the performance index is of the form (2) with $g(x,u) = x_2$.

Table 1 summarizes the parameter values used in the simulations as well as the optimal equilibrium of the system, which corresponds to maximal $x_2$ under constant-input operation.

Fig. 1 depicts the equilibrium curve and the optimal equilibrium point for the CSTR system (18) with the parameter values from Table 1.

Table 1. Parameter values and optimal equilibrium for the CSTR system

<table>
<thead>
<tr>
<th>Parameter Value</th>
<th>Parameter Value</th>
<th>Optimal Equilibrium</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a = 2$</td>
<td>$u^0 = 2\sqrt{2} = 2.5198420997$</td>
<td>$x_1^0 = \frac{\sqrt{9 + 8\sqrt{2}} - 3}{4\sqrt{2}} = 0.2714443171$</td>
</tr>
<tr>
<td>$\beta = 1$</td>
<td>$x_2^0 = \left(\frac{\sqrt{9 + 8\sqrt{2}} - 3}{8\sqrt{2}}\right)^2 = 0.1856670492$</td>
<td></td>
</tr>
<tr>
<td>$\rho = 3/4$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

In what follows, the results of the previous Sections are applied to the CSTR system (18), for both sine wave and square wave input functions. Because on physical grounds the input $u$ needs to be strictly positive, feasible values of the amplitude $M$ are necessarily below $u^0 \approx 2.5$. Maple is used to perform the symbolic computations for the series solution of the Center Manifold Equation, followed by calculation of the integral in the performance index.

6.1. Sine wave input

The effect of a sine wave input $u = M \sin \omega t$, which corresponds to $h(z) = M \cdot z_1$, is first studied for the CSTR system under consideration.

The coefficient of the quadratic term in the expansion (17) (pi criterion) is found to be

$$
\pi(\omega) = \frac{3}{256} \frac{(\sqrt{9 + 8\sqrt{2}} - 3)^2}{\sqrt{9 + 8\sqrt{2}}} \frac{\omega^2 - (9 + 8\sqrt{2})}{\omega^2 + (9 + 8\sqrt{2})} = 0.0050207367 \frac{\omega^2 - 19.0793684}{\omega^2 + 19.0793684}
$$

which is equivalent to the result reported by Sterman & Ydstie [19] for the same system.

All the coefficients of the expansion (17) are rational functions of $\omega^2$. In particular, setting $R = \sqrt{9 + 8\sqrt{2}}$, the expressions for the leading coefficients can be written as follows:

$$
\pi(\omega) = \frac{3}{256} \frac{(R - 3)^2}{R^2} \frac{N_\pi(\omega)}{\omega^2 + R^2}
$$

$$
\rho(\omega) = \frac{3}{256} \frac{2^{1/3}(R - 3)^2}{2^{15}R^3} \frac{N_\rho(\omega)}{(\omega^2 + R^2)^3(4\omega^2 + R^2)}
$$

$$
\sigma(\omega) = \frac{9}{256} \frac{2^{2/3}(R - 3)^2}{2^{22}R^5} \frac{N_\sigma(\omega)}{(\omega^2 + R^2)^3(4\omega^2 + R^2)^2(9\omega^2 + R^2)}
$$

etc.

with the numerator polynomials given by

$$
N_\pi(\omega) = \omega^2 - R^2
$$

$$
N_\rho(\omega) = (180R^2 + 96R + 144)\omega^6 + (873R^4 - 156R^3 + 774R^2)\omega^4 + (579R^6 - 132R^5 - 198R^4)\omega^2 + (-413R^8 + 156R^7 + 90R^6)\omega^2 + (-203R^{10} + 36R^9 + 54R^8)
$$

$$
N_\sigma(\omega) = (180R^2 + 96R + 144)\omega^6 + (873R^4 - 156R^3 + 774R^2)\omega^4 + (579R^6 - 132R^5 - 198R^4)\omega^2 + (-413R^8 + 156R^7 + 90R^6)\omega^2 + (-203R^{10} + 36R^9 + 54R^8)
$$
\[ N_\sigma(\omega) = (477360R^4 + 233280R^3 + 381024R^2 + 186624R \\
+ 279936)\omega^{16} + (3145080R^6 + 1392640R^5 \\
+ 2053968R^4 + 1070496R^3 + 1605744R^2)\omega^{14} \\
+ (8946507R^8 - 134612R^7 + 8595294R^6 \\
- 821016R^5 + 1520496R^4 + 2558016R^3)\omega^{12} \\
+ (12400146R^{10} - 4149768R^9 + 10214460R^8 \\
- 1620000R^7 - 797040R^6)\omega^{10} \\
+ (7446205R^{12} - 2388316R^{11} + 1233282R^{10} + 218376R^9 \\
- 1392640R^8 + 233280R^7 + 381024R^6)\omega^8 \\
+ (8946507R^8 - 134612R^7 + 8595294R^6 \\
- 821016R^5 + 1520496R^4 + 2558016R^3)\omega^6 \\
+ (12400146R^{10} - 4149768R^9 + 10214460R^8 \\
- 1620000R^7 - 797040R^6)\omega^4 \\
+ (7446205R^{12} - 2388316R^{11} + 1233282R^{10} + 218376R^9 \\
- 1392640R^8 + 233280R^7 + 381024R^6)\omega^2 \\
+ (12400146R^{10} - 4149768R^9 + 10214460R^8 \\
- 1620000R^7 - 797040R^6) \text{ etc.} \]

Plots of the coefficients \( \pi(\omega) \), \( \rho(\omega) \), \( \sigma(\omega) \), \( \ldots \) of \( M^2, M^4, M^6, \ldots \) in the expansion (17) are given in Fig.2, in a logarithmic diagram.

Figures 3–4 depict the estimated performance index \( J \) as a function of \( \omega \), when \( M = 1 \) for different approximation orders. In Figures 5–6 the numerical integration curve is compared to the 2nd-order approximation (pi criterion) and to the 12th order approximation of \( J \) derived from our method. It is seen that the 2nd-order approximation (pi criterion) is very accurate compared to the numerical simulation, whereas the higher-order corrections only slightly improve accuracy.

However, for an amplitude of \( M = 2 \), the 2nd order approximation (pi criterion) is no longer accurate in predicting the performance improvement. The addition of higher order corrections provides a definite improvement in accuracy, achieving agreement with the numerical simulation results, as shown in Figures 7–10.

From the point of view of applications, one important parameter is the critical frequency, at which \( J - J_0 \) changes sign; operation above this frequency will result in an improvement of performance for the CSTR. Critical frequency depends on the amplitude, as can be seen by comparing Figures 6 and 10. The pi criterion can only predict...
the low-amplitude limit of the critical frequency. Table 2 compares the values of the critical frequency for 2nd to 12th order approximations when $M = 2$. It is seen that the pi criterion overestimates the critical frequency and underestimates the magnitude of performance improvement for larger $\omega$.

### 6.2. Square wave input

The effect of a square wave input on the reaction system was approximated by using the Fourier series of the square wave up to the third term (see equation (10) with $p = 5$):

$$u \approx M \cdot \frac{4}{\pi} \left( \sin \omega t + \frac{\sin 3\omega t}{3} + \frac{\sin 5\omega t}{5} \right)$$

<table>
<thead>
<tr>
<th>Critical Frequency</th>
<th>$I - I_0$ for $\omega = 0$</th>
<th>$I - I_0$ for $\omega = 30$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2nd order</td>
<td>4.37</td>
<td>-0.0049997</td>
</tr>
<tr>
<td>4th order</td>
<td>4.14</td>
<td>-0.0073460</td>
</tr>
<tr>
<td>6th order</td>
<td>4.04</td>
<td>-0.0082943</td>
</tr>
<tr>
<td>8th order</td>
<td>4.00</td>
<td>-0.0086898</td>
</tr>
<tr>
<td>10th order</td>
<td>3.99</td>
<td>-0.0088607</td>
</tr>
<tr>
<td>12th order</td>
<td>3.98</td>
<td>-0.0089496</td>
</tr>
</tbody>
</table>
Fig. 9. Comparison of the various calculation methods for the Performance Index, for $M = 2$.

Fig. 10. Detail of Fig. 9.

The corresponding $h(z)$ function is

$$h(z) = M \cdot \frac{4}{15\pi} (48z_1^5 - 80z_1^3 + 45z_1)$$

Figures 11–12 depict the estimated performance index $J$ as a function of $\omega$, when $M = 0.6$, for different approximation orders. It is seen that the 2nd order approximation is a poor approximation, whereas higher-order corrections provide improvements. However, because of the alternating pattern of convergence, convergence is relatively slow and it is necessary to go to high orders (12th) in order to obtain an accurate approximation.

In Figures 13–14, the numerical integration curves from both the Fourier approximation and the exact square wave are compared to the 2nd order approximation and to the 12th order approximation of $J$ derived from our method. It is clear that the 2nd order approximation diverges significantly...
Comparing the results under square wave input to the ones under sine wave input, it is seen that, even though the methodology is the same and the nature of the results is similar, convergence in the square wave case is significantly slower. Approximation order of 12 was more than enough in the sine wave case, but barely sufficient in the square wave case.

6.3. Time Responses

Figure 15 depicts the time responses of the system under the studied input functions (sine wave and approximate square wave) for two different amplitudes ($M = 1.0$ and $2.0$) and a fixed frequency $\omega = 25$. The optimal equilibrium point was used as the initial condition.

As expected, the system reaches the Center Manifold (steady cycling) after a small number of periods. The average value of the performance index is higher than the steady-state corresponding to the optimal constant input.

7. Concluding Remarks

An approximate calculation method was developed for the prediction of performance of a nonlinear system under periodic forcing. The proposed method constructs analytical predictions of the performance index as a function of the amplitude and the frequency of the periodic input.

The Pi criterion of Bittanti et al. [7] was generalized in the sense that it represents the 2nd-order term of the derived power series expansion of $J$ with respect to the amplitude. Therefore, the incorporation of higher order terms can significantly improve accuracy under large amplitudes. Furthermore, while the function $\pi(\omega)$ supplies a range of frequencies within which performance improvement is possible, the proposed method approximates the performance index itself, thus capturing the effect of both frequency and amplitude on the magnitude of the performance criterion. The derived approximate formula for the performance index is therefore useful for optimization, for the purpose of selecting the optimal frequency and amplitude of periodic operation.

It was shown that the calculation of higher order correction terms to the performance index is theoretically possible and also, computationally feasible, with the use of a symbolic programming application (Maple). The truncation order for satisfactory convergence depends on the type of the input and the state equations. The presence of multiple harmonics in the input and/or strong nonlinearities in the dynamic model necessitates the calculation of higher order terms, in order to obtain an accurate approximation.

Future research will need to deal with computational complexity issues, so that the proposed approach can be effective in handling more complex application problems. An analysis of the inherent computational complexity of the operations involved in the calculations will be needed. In addition, symbolic programming needs to be optimized, in the sense of
Fig. 15. Time responses for sine wave input and approximate square wave input, with amplitudes $M = 1.0$ and $M = 2.0$ and frequency $\omega = 25$.

being tailored to the specific calculations involved. Automatic differentiation or related techniques can be helpful in this direction.

Acknowledgement

Financial support from a C. Karatheodory Grant of the University of Patras is gratefully acknowledged.

References

11. Dermitzakis I, Kravaris C. Higher-Order Corrections to the $\Pi$ Criterion for the Periodic Operation of Chemical Reactors,
Proceedings of the 3rd IEEE Multi-conference on Systems and Control, St. Petersburg, Russia, 2009, 376–381.


