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Parametric optimization of digitally controlled nonlinear reactor dynamics using Zubov-like functional equations

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The present work aims at the development of a systematic method to optimally choose the parameters of digitally controlled nonlinear reactor dynamics. In addition to traditional performance requirements for the controlled reactor dynamics such as stability, fast and smooth regulation, disturbance rejection, etc., optimality is requested with respect to a physically meaningful performance. The value of the performance index is analytically calculated via the solution of a Zubov-like functional equation and becomes explicitly parameterized by the digital controller parameters. A standard static optimization algorithm yields subsequently the optimal values of the above parameters. Within the proposed framework, stability region estimates are also provided through the solution of the above functional equation. Finally, a nonlinear chemical reactor example following Van de Vusse kinetics is used in order to illustrate the proposed parametric optimization method.

KEY WORDS: chemical reaction system dynamics, nonlinear dynamics, parametric optimization, functional equations, Lyapunov stability

1. Introduction

In recent years, the development of powerful analytical and computational tools enabled the analysis of the dynamic behavior of complex nonlinear chemical reaction systems to be performed in a thorough and rigorous manner [1–4]. As a result, the "inverse problem" of modifying and controlling the above dynamic behavior has also received considerable attention [5,6]. In particular, it is widely recognized that quite often the chemical reactor dynamics is often driven by "input" variables associated with the reactor feeding and reaction initiation policy (feed flow rates, reactant inlet concentration, etc.), and therefore it is amenable to modification through feedback action and the subsequent enforcement of the desirable dynamic modes and behavior [5,6]. Equivalently stated, one

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may derive a feedback control law that dictates the appropriate input profile, which in turn, enforces the requisite and desirable dynamic behavior on the controlled reactor dynamics. In particular, unexpected disturbances may occur driving the chemical reactor far from the design steady state conditions, and the primary objective is to derive a control law capable of driving the system back to the design steady-state in a smooth, fast and reliable manner, thus rejecting the disturbance effect [5,6]. The above represents a typical scenario of a reactor regulation problem that can be adequately addressed via the action of a feedback controller. Please notice, that a feedback regulator enjoys design flexibility by introducing tunable controller parameters that can be adjusted in order to assign the desirable dynamic characteristics to the controlled reactor dynamics (speed and non-oscillatory characteristics of the reactor's response, tolerable overshoot, size of the stability region, transient behavior towards the stable manifold, as well as other asymptotic properties) [5,7]. Over the last two decades significant research effort has concentrated on the nonlinear feedback controller synthesis problem, in order to overcome performance limitations associated with linear controller design methods applied to linearized reactor dynamic models [5,7]. Furthermore, the advent of digital technology revolutionized the way advanced nonlinear feedback control algorithms are implemented in practice with the aid of a computer. Nowadays, computer-based digital control systems are successfully designed and used in a multitude of applications [8,9]. However, the problem of systematically selecting the digital controller parameters for nonlinear chemical reactors has not been given proper attention, and has been traditionally addressed either through heuristics or trial-and-error type of approaches, thus inevitably resorting to extensive dynamic simulations and/or costly experiments [9,10]. The proposed approach aims at the development of a systematic and comprehensive method to optimally select the parameters of a nonlinear digital reactor control system, when in addition to standard performance requirements of the controlled reactor dynamics (stability, fast and smooth regulatory response and disturbance rejection), optimality is also requested with respect to a physically meaningful performance index. In the present study, the tunable parameters of the feedback controlled reactor dynamics are optimally selected through the minimization of a performance index, representing the decision variables of the associated optimization problem. Under this formulation, the problem under consideration becomes a finite-dimensional static optimization problem, as opposed to an infinite-dimensional nonlinear optimal control problem that could exhibit computational challenges in practice [11]. Traditionally, the above optimization problem is carried out in a "brute force" manner: after an initial guess for the controller parameters, the dynamic equations of the controlled reactor dynamics are simulated and the value of the performance functional is calculated numerically. Then, a gradient-direction method is typically applied to update the controller parameter values until convergence of the recursive algorithm leads to an optimal set of controller parameter values [11]. More elaborate methods

from an algorithmic and computational point of view have also appeared in the pertinent body of literature. They rely either on numerical techniques for solving challenging two-point boundary value problems, or large scale nonlinear mathematical programs resulting from time-discretization and parameterization of the input variables [11,12].

The present research study introduces a systematic and practical methodology that addresses the above finite-dimensional static parametric optimization problem for digitally controlled nonlinear reactor dynamics. In particular, the proposed approach is based on the explicit calculation of a physically meaningful quadratic performance index by solving a Zubov-like functional equation. It can be proven that the functional equation admits a unique locally analytic solution in the vicinity of the reference equilibrium point, which is also endowed with all the properties of a Lyapunov function for the controlled reactor dynamics. Therefore, a transparent and very useful link between optimality and stability can be established through the solution of the above functional equation. Furthermore, the analyticity of the solution enables the development of a series solution method for the functional equation that can be easily implemented with the aid of a symbolic software package such as MAPLE. It is also shown that the evaluation of the above Lyapunov function solution at the initial conditions leads to an explicit calculation of the value of the performance index. Since the dynamic equations of the controlled reactor dynamics are parameterized by the controller parameters, the Lyapunov function and solution to the functional equation is also parameterized, and therefore, the value of the performance index depends explicitly on the controller parameters. In light of the above observation, the employment of static optimization techniques can provide the optimal values of the finite set of controller parameters. Moreover, it should be pointed out, that for the optimally calculated controller parameter values, an explicit estimate of the size of the system's stability region can also be provided by using results from advanced stability theory for discrete dynamical systems [13,14].

The present paper is organized as follows: In Section 2 a succinct description of the requisite mathematical preliminaries and background is provided. Section 3 encompasses the main ideas and algorithmic structure of the proposed approach for parametric optimization of nonlinear digitally controlled reactor dynamics. In Section 4 simulation studies have been conducted in a representative chemical reactor example in order to evaluate the proposed method and illustrate its applicability. Finally, a few concluding remarks are provided in Section 5.

2. Mathematical preliminaries and motivation

Before we embark on the presentation of the proposed parametric optimization scheme for nonlinear digitally controlled reactor dynamics, let's first consider the simpler case of linear reactor dynamics in order to conceptually and

methodologically motivate the development of its nonlinear analogue. The latter represents the focus of the present study.

A linear (or linearized) autonomous dynamic system is considered in the discrete-time domain:

$$x(k+1) = Ax(k) \tag{1}$$

where the non-negative integer $k \in \aleph = \{0, 1, 2, \dots\}$ is the discrete time index, $x(k) \in \Re^n$ is the vector of state variables at the time instant k and A an $n \times n$ constant matrix. The above linear dynamic system in the discrete-time domain represents the linear discrete dynamics of a chemical reactor that is obtained either:

a. through a reliable and accurate discretization method applied to the original continuous-time reactor dynamics in order to digitally (numerically) simulate the dynamic behavior of the reactor of interest [5,9,15]

or:

b. through direct system identification methods and a set of historical input/output data, in the case where the reactor dynamics and the associated kinetics are discouragingly complex and not amenable to first-principle based modeling [5,9]. In both cases however, it is assumed that (1) adequately captures the actual linear reactor dynamics.

It is also assumed that the above system's characteristic matrix A has stable eigenvalues, which were assigned thanks to a fixed structure linear controller, designed in accordance to well-known methods [7,9].

The following quadratic performance index associated with system (1) can be defined:

$$J = \sum_{k=0}^{\infty} [x(k)]^T \, Q \, [x(k)] \tag{2}$$

where Q is an arbitrarily selected positive-definite symmetric matrix, and the superscript T denotes the transpose of a vector or a matrix. Notice, that the aforementioned stability requirement on the reactor dynamics (1) implies that the infinite series in (2) converges to a fixed value limit J [13,14].

Introducing the following Lyapunov matrix equation:

$$A^T P A - P = -Q \tag{3}$$

one can easily show that equation (3) admits a unique symmetric and positive-definite solution P [13]. Furthermore, applying standard Lyapunov stability theorems [13], it can be inferred that the quadratic form defined as:

$$V(x) = x^T P x \tag{4}$$

has the following properties:

$$V(x) > 0, V(0) = 0$$

$$\Delta V\,(x\,(k)) = V(x(k+1)) - V(x(k)) = -x\,(k)^T\,Qx\,(k) < 0 \tag{5}$$

and therefore, it qualifies as a Lyapunov function [13].

Using equation (5) one obtains:

$$\begin{aligned} J &= \sum_{k=0}^{\infty} [x(k)]^{\,T} Q\,[x(k)] = -\sum_{k=0}^{\infty} [V\,(x(k+1)) - V\,(x(k))] \\ &= V\,(x(0)) - V\,(x(\infty)) = V\,(x(0)) \end{aligned} \tag{6}$$

since$V\,(x\,(\infty)) = V\,(x\,(k \to \infty)) = V\,(0) = 0$ due to the aforementioned stability assumption [13,14].

Therefore, the value of the performance index J can be easily calculated through the formula below:

$$J = V(x(0)) = [x(0)]^T\,P\,[x(0)] \tag{7}$$

where P is the unique solution of the Lyapunov matrix equation (3) and $x(0)$ the initial value of the state vector.

Please notice, that the interesting feature of this approach is signified by the underlying connection between optimality (performance index) and stability (Lyapunov function). This link was first explored and mathematically established by Bertram and Kalman [10] in the continuous time domain.

Let us now examine how the above ideas and techniques can be generalized in order to account for nonlinear dynamics.

Nonlinear reactor dynamics in the discrete time domain are considered:

$$x(k+1) = \varphi(x(k)) \tag{8}$$

where $x(k) \in \Re^n$ is the vector of state variables at the discrete time instant k and $\varphi(x)$ a real analytic vector function defined on $\Re^n$. Let x_0 be the reference (fixed) equilibrium point of interest:

$$\varphi(x_0) = x_0. \tag{9}$$

As it was mentioned in the linear reactor dynamics case, the discrete reactor dynamics and nonlinear difference equations (8) are assumed to have been obtained either through an accurate and reliable discretization method for the numerical (digital) simulation of the original continuous-time reactor dynamics, or through standard system identification methods [5,7–9,15]. It should be emphasized that the state space representation of the reactor dynamics (8) in the discrete time domain (realized via a nonlinear system of difference equations)

represents the point of departure of any meaningful study of the digital reactor monitoring and control system design problem [9].

Furthermore, as in the linear case, let us assume that a fixed structure feedback controller has been designed, so that (8) represents the control reactor dynamics that has been rendered locally asymptotically stable. This is equivalent to assume that the Jacobian matrix of the linearized system $A = \frac{\partial \varphi}{\partial x}(x_0)$ has stable eigenvalues, i.e. eigenvalues that all lie inside the unit disc on the complex plane [9].

In this case, a quadratic performance index or cost function can be defined as follows:

$$J = \sum_{k=0}^{\infty} Q(x(k)) \tag{10}$$

where $Q(x)$ is an arbitrarily selected positive-definite real analytic scalar function defined on $\Re^n$ with $Q(x_0) = 0$ and $\frac{\partial Q}{\partial x}(x_0) = 0$.

Let us now introduce the following functional equation:

$$V(\varphi(x)) - V(x) = -Q(x) \tag{11}$$

accompanied by the boundary condition:

$$V(x_0) = 0$$

where the unknown solution is a scalar function $V(x)$ with $V : \Re^n \to \Re$. One easily observes:

$$J = \sum_{k=0}^{\infty} Q(x(k)) = -\sum_{k=0}^{\infty} [V(x(k+1)) - V(x(k))] = V(x(0)) - V(x(\infty)) \tag{12}$$

and since $V(x(\infty)) = V(x(k \to \infty)) = V(x_0) = 0$ due to the stability assumption stated earlier, the following equality can be established:

$$J = V(x(0)) \tag{13}$$

Therefore, the above ideas allow a direct and explicit calculation of the value of the performance index in terms of the solution of the functional equation (11), assuming it exists and can be computed.

Moreover, we are provided with some interesting properties concerning the solution $V(x)$ of the functional equation (11). Notice that by construction, the rate of change $\Delta V(x(k))$ is negative definite since $Q(x)$is positive definite:

$$\Delta V(x(k)) = V(\varphi(x(k))) - V(x(k)) = -Q(x(k)) < 0 \tag{14}$$

and therefore, if the solution of the functional equation (11) can be proven to be positive definite, it also qualifies as a Lyapunov function for the controlled reactor dynamics (8) [13]. In such a case, the stability property of dynamics (8) and standard converse Lyapunov stability theorems for nonlinear discrete dynamical systems [13] imply the existence of a Lyapunov function that satisfies the functional equation (11). It should be emphasized, that the above construction represents exactly the discrete-time analogue of Zubov's PDE that was developed for the explicit computation of Lyapunov functions for nonlinear dynamical systems modeled through ODEs in the continuous-time domain [14,16]. With respect to the above Zubov-like functional equation (11) the following important issues need to be addressed:

2.1. *Existence and uniqueness of solution*

Theorems in references [14,17–19] guarantee the existence and uniqueness of a locally analytic solution $V(x)$ of the functional equation (11) in the vicinity of the reference equilibrium point x_0.

2.2. *Solution method*

From a practical point of view, one needs to develop a comprehensive method for solving the functional equation (11). Since $\varphi(x)$, $Q(x)$ and the solution $V(x)$ are locally analytic, it is possible to calculate the solution $V(x)$ as a multivariate Taylor series around the equilibrium point of interest $x = x_0$.

The proposed solution method can be realized through the following steps:

a. Expand $\varphi(x)$, $Q(x)$ and the unknown solution $V(x)$ in multivariate Taylor series and insert them into functional equation (11).

b. Equate the Taylor coefficients of the same order of both sides of functional equation (11)

c. Derive a hierarchy of linear recursion formulas through which one can calculate the Nth order coefficient of $V(x)$ given the Taylor coefficients up to order $N-1$ that have been computed in previous recursive steps.

It is feasible to explicitly derive the aforementioned recursive formulas and present them in a mathematically compact form if tensorial notation is used [18]:

a. The partial derivatives of the $\mu - th$ component $f_\mu(x)$ of a vector function $f(x)$ evaluated at $x = x_0$ are denoted as follows:

$$f_{\mu}^{i} = \frac{\partial f_{\mu}}{\partial x_i}(x_o)$$
$$f_{\mu}^{ij} = \frac{\partial^2 f_{\mu}}{\partial x_i \partial x_j}(x_o) \tag{15}$$
$$f_{\mu}^{ijk} = \frac{\partial^3 f_{\mu}}{\partial x_i \partial x_j \partial x_k}(x_o), \text{ etc} \ldots$$

b. The standard summation convention where repeated upper and lower tensorial indices are summed up.

Under the above notation, the unknown solution $V(x)$ of the functional equation (11) represented as a multivariate Taylor series attains the following form:

$$V(x) = \frac{1}{1!} V^{i_1} \left(x_{i_1} - x_{i_{1,0}}\right) + \frac{1}{2!} V^{i_1 i_2} \left(x_{i_1} - x_{i_{1,0}}\right) \left(x_{i_2} - x_{i_{2,0}}\right) + \ldots$$
$$+ \frac{1}{N!} V^{i_1 i_2 \ldots i_N} \left(x_{i_1} - x_{i_{1,0}}\right) \ldots \left(x_{i_N} - x_{i_{N,0}}\right) + \ldots \tag{16}$$

As mentioned above, one inserts the Taylor series expansions of $\varphi(x)$, $Q(x)$, $V(x)$ into functional equation (11) and starts equating coefficients of the same order.

Since $Q(x_0) = \frac{\partial Q}{\partial x}(x_0) = 0$, one can easily show that $V(x)$ does not have linear terms in x : $\frac{\partial V}{\partial x}(x_0) = 0$, or equivalently $V^{i_1} = 0$ for $i_1 = 1, \ldots, n$.

Furthermore, the following relation for the N-th order coefficients can be obtained:

$$\sum_{L=1}^{N} \sum_{\substack{0 \leqslant m_1 \leqslant \ldots \leqslant m_L \\ m_1 + m_2 + \ldots + m_L = N}} V^{j_1 \ldots j_L} \varphi_{j_1}^{m_1} \ldots \varphi_{j_L}^{m_L} = -Q^{i_1 \ldots i_N} \tag{17}$$

where $i_1, \ldots, i_N = 1, \ldots, n$ and $N \geqslant 2$. Note that the second summation symbol in the above formula indicates summing up the relevant quantities over the $\frac{N!}{m_1! \ldots m_L!}$ possible combinations to assign the N indices $(i_1, \ldots, i_N)$ as upper indices to the L positions $\varphi_{j_1}, \ldots, \varphi_{j_L}$, with m_1 of them being put in the first position, m_2 of them in the second one , etc $\left(\sum_{i=1}^{L} m_i = N\right)$ [18].

Please notice that the above expression represents a set of *linear* algebraic equations in the unknown coefficients $V^{i_1, \ldots, i_N}$. This is precisely the mathematical reason that enables the proposed method to be easily implemented using a symbolic software package. Indeed, a simple and comprehensive MAPLE code has been developed to automatically compute the Taylor coefficients of the unknown solution $V(x)$ of the Zubov-like functional equation (11) (see Appendix).

2.3. Local positive definiteness of the solution $V(x)$

Let

$$\varphi(x) = x_0 + A\,(x - x_0) + \overline{\varphi}(x) \tag{18}$$

and

$$Q(x) = (x - x_0)^T\, Q\,(x - x_0) + \overline{Q}(x) \tag{19}$$

with $\overline{\varphi}(x)$, $\overline{Q}(x)$ real analytic and

$$\overline{\varphi}(x_0) = \overline{Q}(x_0) = \frac{\partial \overline{\varphi}}{\partial x}(x_0) = \frac{\partial \overline{Q}}{\partial x}(x_0) = 0 \tag{20}$$

Furthermore, one may represent the solution $V\,(x)$ of (11) as follows:

$$V(x) = (x - x_0)^T\, P\,(x - x_0) + \overline{V}(x) \tag{21}$$

where

$$\overline{V}(x_0) = \frac{\partial \overline{V}}{\partial x}(x_0) = \frac{\partial^2 \overline{V}}{\partial x^2}(x_0) = 0 \tag{22}$$

It can be easily shown that matrix P satisfies the following Lyapunov matrix equation:

$$A^T P A - P = -Q \tag{23}$$

which coincides with the one encountered in the linear case (equation 3). Under the assumptions stated, the above matrix equation admits a unique, positive-definite and symmetric solution P, and therefore, $V(x)$ is locally positive definite and a Lyapunov function for the controlled reactor dynamics (8) [13].

2.4. Stability region estimates

Let N be the truncation order corresponding to an Nth order Taylor polynomial approximation $V^{(N)}\,(x)$ of the solution of the Zubov-like functional equation (11).

Let

$$\Omega^{(N)} = \left\{ x \in \Re^n | x \neq x_0 \wedge \Delta V\,(x) = 0 \right\} \tag{24}$$

and

$$C^{(N)} = \min_{x \in \Omega^{(N)}} V^{(N)}(x) \tag{25}$$

Then, thanks to standard Lyapunov stability theorems for nonlinear discrete-time systems, the set $S^{(N)}(x)$ defined below can be proven to be wholly contained in the stability region of system (8) [13]:

$$S^{(N)}(x) = \left\{ x \in \Re^n | V^{(N)}(x) \leqslant C^{(N)} \right\} \tag{26}$$

Therefore, the set $S^{(N)}(x)$ represents an estimate of the system's stability region. [13,14].

3. The proposed approach

The link established in the previous section between optimality and reactor stability through a Lyapunov function satisfying a Zubov-like functional equation can adequately serve the purposes of optimally choosing the parameters of a digital control system with respect to a performance index. In particular, the optimal selection of the digital controller parameters can be attained through the static optimization of the performance index, whose value is explicitly calculated through the solution of the functional equation that is now parameterized by the controller parameters.

Let us consider the following nonlinear discrete-time dynamical system with a state space representation describing the input-driven reactor dynamics:

$$x(k+1) = \varphi(x(k), u(k)) \tag{27}$$

where

- $k = 0, 1, \ldots$ is the discrete time index
- $u \in \Re$ is the input variable (typically being the feed flow rate, or the inlet reactant concentration, or the temperature of the feed stream, etc.) that can be manipulated according to a "control law" that modifies the reactor dynamics and enforces the desired dynamic behavior [5,7,8,20]
- $x(k) \in \Re^n$ is the vector of state variables
- $\varphi(x, u(x))$ and $h(x)$ are real analytic functions defined on $\Re^n \times \Re$ and $\Re^n$ respectively,

Without loss of generality, it is assumed that the origin $x_0 = 0$ is the reference equilibrium point that corresponds to: $u = u_0 = 0 : \varphi(0, 0) = 0$.

A typical scenario of a reactor regulation problem presupposes that exogeneous disturbances unexpectedly occurred driving the system far from the design steady state conditions. The control objective is to derive a control law that would dictate the requisite pattern of manipulating the input variable u , modify the reactor dynamics in a desirable fashion (the reactor dynamics is driven by u) and bring the system back to the design steady state, thus rejecting the effect of

the disturbances. There is a variety of well-performing and carefully synthesized nonlinear reactor regulation laws in the pertinent body of literature [5,7,9], and the simplest of which exhibits the following structure:

$$u(k) = \kappa\,(x\,(k)\,;\,p) \tag{28}$$

where $p \in P$ represents the m -dimensional vector of controller parameters and P the admissible parameter space, which is assumed to be a compact subset of $\Re^m$. Furthermore, $\kappa\,(x;\,p)$ is assumed to be a real analytic scalar function, defined on $\Re^n \times P$, with $\kappa\,(0;\,p) = 0$.

It should be pointed out, that all system regulation laws introduce a set of controller parameters $p \in P$ [5,7,9]. The latter reflect the controller degrees of freedom (the controller design flexibility). Indeed, the controller parameters are selected in such a manner that the desired dynamic behavior is assigned to the controlled reactor dynamics by the regulator. Desirable characteristics would be a stable, non-oscillatory and relatively fast response/reversion to the design steady state in the presence of disturbances, suppressing intolerable overshoots, or meeting certain optimality criteria [5,7,9]. Traditionally, the selection of the nonlinear regulator parameters p has been achieved through heuristics or trial-and-error type of approaches [7,9]. In the context of the present study however, p would be optimally selected through the optimization of a physically meaningful performance index and the ideas presented in the previous section.

The controlled (regulated) reactor dynamics can be easily obtained by inserting (28) into the reactor dynamics equation (27):

$$x\,(k+1) = \varphi\,(x\,(k)\,,\kappa\,(x\,(k)\,;\,p)) \tag{29}$$

Let

$$\begin{aligned} J(p) &= \sum_{k=0}^{\infty} \left\{\, \|x(k)\|^2 + \rho\,\|u(k)\|^2 \right\} \\ &= \sum_{k=0}^{\infty} \left\{\, \|x(k)\|^2 + \rho\,\|\kappa\,(x\,(k)\,;\,p)\|^2 \,\right\} \end{aligned} \tag{30}$$

The choice of the above quadratic performance index is physically meaningful and can be justified by the fact that it contains a term: $\|x(k)\|^2$ that captures the distance of the current dynamic reactor state from the reference equilibrium point (assumed to be the origin) as the regulator forces the reactor to asymptotically reach it, and a second one: $\|u(k)\|^2$ that represents a measure of the necessary control effort in order to successfully perform the system's regulation at the origin.

Please notice, that since the regulation law introduces the parameters p, the performance index J will depend on p as well.

To simplify the notation, let us define the vector function $\Phi(x(k); p) = \varphi(x(k), \kappa(x(k); p))$ and the positive definite scalar function $Q(x(k); p) = \|x(k)\|^2 + \rho \|\kappa(x(k); p)\|^2$.

Under the above notation, the controlled reactor dynamics (29) and the performance index $J(p)$ can be rewritten as follows:

$$x(k+1) = \Phi(x(k); p) \tag{31}$$

$$J(p) = \sum_{k=0}^{\infty} Q(x(k); p) \tag{32}$$

Please notice, that the problem under consideration is now formulated exactly as the one presented in the previous section. However, the dependence of both the controlled system dynamics and the performance index on the controller parameter vector p is now explicit.

As intuitively expected, the regulator (28) has rendered the controlled reactor dynamics stable, and therefore, the Zubov-like functional equation:

$$V(\Phi(x(k)); p) - V(x(k)) = -Q(x; p) \tag{33}$$

admits a unique locally analytic solution $V(x; p)$,which is a Lyapunov function that explicitly depends on the controller parameters p. Moreover, the performance index $J(p)$ is exactly the value of V at the initial state:

$$J(p) = V(x(0); p) \tag{34}$$

Therefore, given an initial condition $x(0)$, the optimal values for the controller parameters p^* can be obtained through the solution of the following finite-dimensional parametric optimization problem:

$$p* = \arg\min_{p \in P} J(p) = \arg\min_{p \in P} V(x(0); p) \tag{35}$$

subject to a set of constraints that guarantee that the Jacobian matrix $\frac{\partial \Phi}{\partial x}(0; p)$ has stable eigenvalues (stability requirement). The above static optimization problem is a nonlinear mathematical program for which a multitude of numerically efficient algorithms and techniques exist in the literature [12]. Furthermore, the set of admissible parameters P and the constraints associated with the reactor stability assumptions render this optimization problem a constrained one. It should be pointed out, that the proposed approach can be computationally demanding under certain circumstances for higher-order large-scale systems due to the formulation of the optimization problem that presupposes the symbolic calculation of the solution of the functional equation (11). However, the comparative advantage of the proposed method is that it allows a more transparent and insightful analysis of the reactor dynamics to be performed, establishing a very important system-theoretic link between stability and a physical measure of

performance such as an optimality criterion [10,14,16]. Furthermore, as it will be seen in the next section's illustrative example, the availability of enhanced computational capabilities naturally generates new interest in the practical application of the above ideas and the proposed optimization scheme.

4. Illustrative example

To illustrate the main aspects and different steps of the proposed algorithmic approach, let us consider the series/parallel Van de Vusse reaction [21] taking place in a continuous stirred tank chemical reactor in isothermal operation [5,6]:

$$\begin{array}{c} A \rightarrow B \rightarrow C \\ 2A \rightarrow D \end{array} \tag{36}$$

with the rates of formation of species A and B given by:

$$r_A = -k_1 C_A - k_3 C_A^2 \tag{37}$$

$$r_B = k_1 C_A - k_2 C_B \tag{38}$$

Under the assumption that the feed stream consists of pure A, the mass balance equations for species A and B lead to the following nonlinear dynamic process model [21]:

$$\begin{aligned} \frac{\mathrm{d}C_\mathrm{A}}{\mathrm{d}t} &= f_1\left(C_\mathrm{A}, C_\mathrm{B}, \frac{F}{V}\right) = \frac{F}{V}\left(C_{A_0} - C_\mathrm{A}\right) - k_1 C_\mathrm{A} - k_3 C_\mathrm{A}^2 \\ \frac{\mathrm{d}C_\mathrm{B}}{\mathrm{d}t} &= f_2\left(C_\mathrm{A}, C_\mathrm{B}, \frac{F}{V}\right) = -\frac{F}{V} C_\mathrm{B} + k_1 C_\mathrm{A} - k_2 C_\mathrm{B} \end{aligned} \tag{39}$$

where F is the inlet flow rate of A, V is the volume of the reactor that is considered to be constant during the operation, C_A and C_B are the concentrations of species A and B in the reactor respectively, and C_{A_0} is the concentration of A in the feed stream. The control objective is to regulate the concentration C_B at a constant desired level (set-point) by manipulating the dilution rate $\left(F/V\right)$.

The above reactor-dynamic model is mathematically represented in the continuous time domain. In order to digitally control and optimize the reactor dynamic behavior a discretization method is needed [5,6,9].

Any type of time-discretization can be used in principle, but for the sake of simplicity let us employ a basic Euler's discretization scheme for the nonlinear ODEs (39). One obtains:

$$\begin{aligned} C_\mathrm{A}(k+1) &= C_\mathrm{A}(k) + \delta f_1\left(C_\mathrm{A}(k), C_\mathrm{B}(k), \left(F/V\right)(k)\right) \\ &= \varphi_1\left(C_\mathrm{A}(k), C_\mathrm{B}(k), \left(F/V\right)(k)\right) \\ C_\mathrm{B}(k+1) &= C_\mathrm{B}(k) + \delta f_2\left(C_\mathrm{A}(k), C_\mathrm{B}(k), \left(F/V\right)(k)\right) \\ &= \varphi_2\left(C_\mathrm{A}(k), C_\mathrm{B}(k), \left(F/V\right)(k)\right) \end{aligned} \tag{40}$$

where k is the discrete-time index, and δ is the discretization time-step. Please notice that the time step δ has been chosen small enough compared to the dominant process time constant in order to avoid a numerical instability. Under the above assumption, it was numerically verified that the nonlinear difference equations (40) capture quite adequately the reactor's actual dynamic behavior.

Let us now consider the problem of optimally calculating the digital controller parameters for a specific step change in the set point. In all ensuing simulation runs the set-point for C_B was chosen to be $C_{B,S} = 1.05$ gmol/l with the corresponding reactor equilibrium state being at:

$$\begin{aligned} \left(F/V\right)_S &= 28.428\text{h}^{-1} \\ C_{A_s} &= 2.697\text{gmol/l} \\ C_{B_s} &= 1.05\text{gmol/l} \end{aligned}$$

In order to conform to the theory presented in previous sections and facilitate the pertinent calculations, deviation variables with respect to the above reference steady state are defined as follows:

$$x_1(k) = C_A(k) - C_{A_s}, x_2 = C_B(k) - C_{B_s}, u = (F/V)(k) - (F/V)_S \tag{41}$$

Notice, that the origin becomes now the reference equilibrium point when deviation variables are used.

Using the above set of deviation variables the reactor dynamic model can be put in the following form:

$$\begin{aligned} x_1(k+1) &= \overline{\varphi_1}(x_1(k), x_2(k), u(k)) \\ x_2(k+1) &= \overline{\varphi_2}(x_1(k), x_2(k), u(k)) \end{aligned} \tag{42}$$

with

$$\begin{aligned} \overline{\varphi_1}(x_1(k), x_2(k), u(k)) &= \varphi_1\left(x_1(k) + C_{A_s}, x_2(k) + C_{B_s}, u(k) + \left(F/V\right)_S\right) \\ \overline{\varphi_2}(x_1(k), x_2(k), u(k)) &= \varphi_2\left(x_1(k) + C_{A_s}, x_2(k) + C_{B_s}, u(k) + \left(F/V\right)_S\right) \end{aligned}$$

The numerical values used for the various process parameters are tabulated in Table 1.

Table 1
Numerical values of the process parameters.

Parameter	Value
k_1	10 h^{-1}
k_2	100 h^{-1}
k_3	10 l/gmol/h
C_{A_0}	10 gmol/l

A simple digital linear regulation law was applied to the system:

$$u(k) = -p_1 x_1(k) - p_2 x_2(k) \tag{43}$$

where $\{p_1, p_2\}$ are the regulator parameters to be optimized [9]. According to the proposed method, their optimal values can be obtained by minimizing the following performance index:

$$J(p_1, p_2) = \sum_{k=0}^{\infty} [x_2(k)]^2 + \rho [u(k)]^2 = \sum_{k=0}^{\infty} [x_2(k)]^2 + \rho [p_1 x_1(k) + p_2 x_2(k)]^2 \tag{44}$$

Applying the method described in Sections 2 and 3, the above performance index can be explicitly calculated as follows:

$$J(p_1, p_2) = V(x_1(0), x_2(0); p_1, p_2) \tag{45}$$

where $V(x_1, x_2; p_1, p_2)$ is the solution of the following Zubov-like functional equation:

$$\begin{aligned} &V(\overline{\varphi}_1(x_1, x_2, -p_1 x_1 - p_2 x_2), \overline{\varphi}_2(x_1, x_2, -p_1 x_1 - p_2 x_2))) - V(x_1, x_2) \\ &\quad = -x_2^2 - \rho (p_1 x_1 + p_2 x_2)^2 \end{aligned} \tag{46}$$

The above functional equation was solved symbolically using the software package MAPLE and the series solution method for a finite truncation order N. The result was evaluated at the chosen initial condition and the function $V^{(N)}(x_1(0), x_2(0); p_1, p_2)$ was minimized using the nonlinear programming library of MAPLE (see Appendix):

$$p^* = \arg\min_{p \in P} J(p_1, p_2) = \arg\min_{p \in P} V^{(N)}(x_1(0), x_2(0); p_1, p_2) \tag{47}$$

The optimal values of p_1 and p_2 for different values of the step size and different orders of truncation N are presented in figures 1 and 2. These values were obtained with a weight coefficient $\rho = 10^{-5}$. Please notice that the step size is a measure of how drastic the disturbance effect has been, driving the system far from the desired final equilibrium state.

As suggested by figures 1 and 2, the optimal values of the regulator parameters p_1 and p_2 are highly dependent on the step size. This is of course intuitively expected due to the nonlinear nature of the system under study. An additional piece of information provided by these figures, is that fast convergence is attained, as the order of series truncation N increases. In this particular case study, an order of truncation $N = 4$ is enough for a satisfactory approximation.

Figures 3 and 4 show the optimal responses obtained with different values of the weight coefficient ρ. As expected, when the weight coefficient ρ

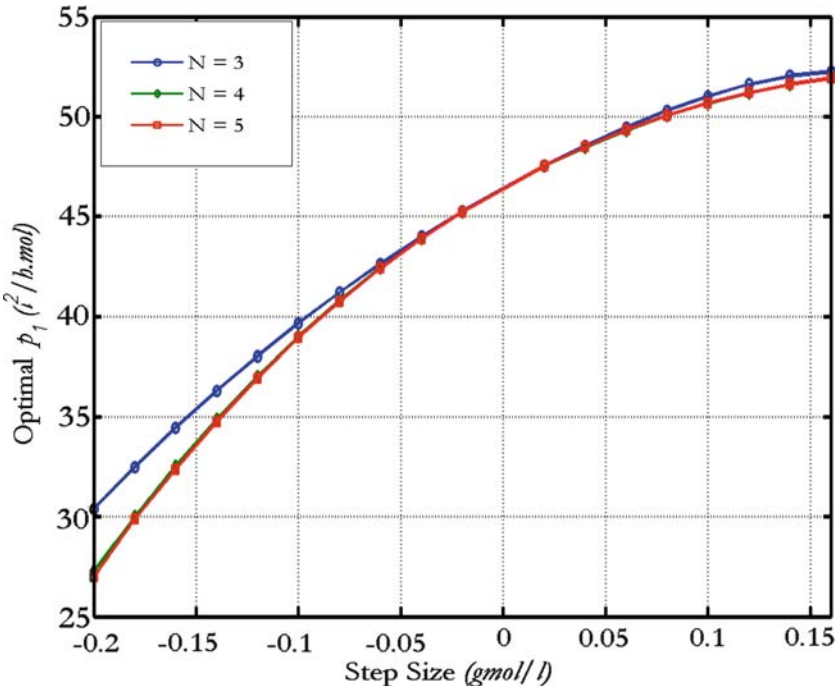

Figure 1. Optimal values of p_1 as a function of the size of the step change in the set point.

attains small values the system's response is very fast, but at the expense of unrealistic values of the dilution rate. Indeed, as we lower the value of ρ , we tend not to drastically penalize the control effort needed for reactor regulation, the regulator becomes more aggressive, the reactor response that it induces faster, but the values of the input variable u that are generated may become physically unrealizable. The opposite effect is naturally observed for larger values of the weight coefficient. In this case, a large control effort u is severely penalized, the regulator becomes less aggressive enforcing a dynamically more sluggish response and reversion to the desired reference equilibrium state.

Finally, figures 5 and 6 illustrate how the method described in Section 2 is used to obtain stability region estimates. This is a very useful feature of the proposed method, because it also equips us with the capacity to assess the reactor's stability characteristics under the optimal regulator parameters. In particular, stability region estimates were obtained by considering the largest contour curve of the function $V(x)$ which is tangent to the $\Delta V^{(N)}(x) = 0$ curve, and wholly contained in the region where $\Delta V^{(N)}(x) < 0$ [14,16].

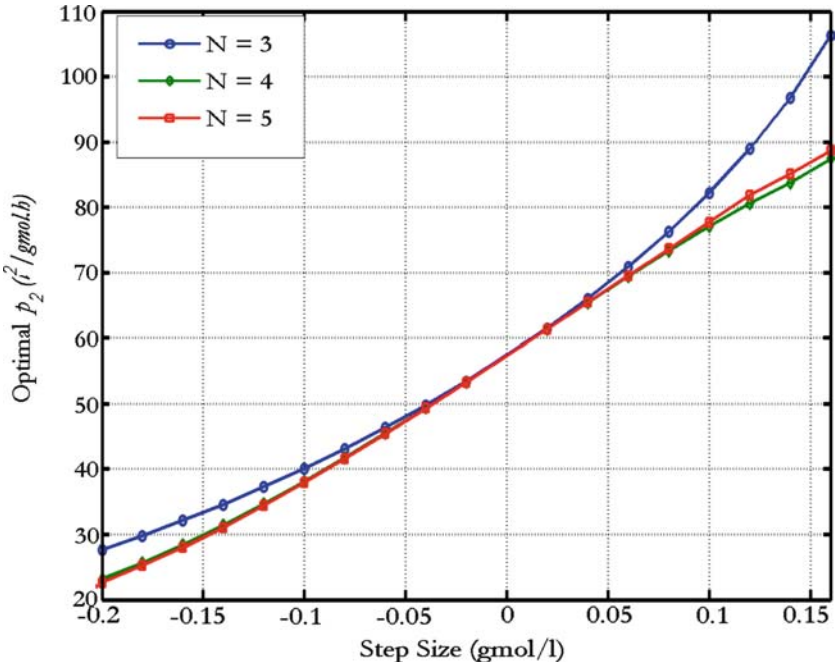

Figure 2. Optimal values of p_2 as a function of the size of the step change in the set point.

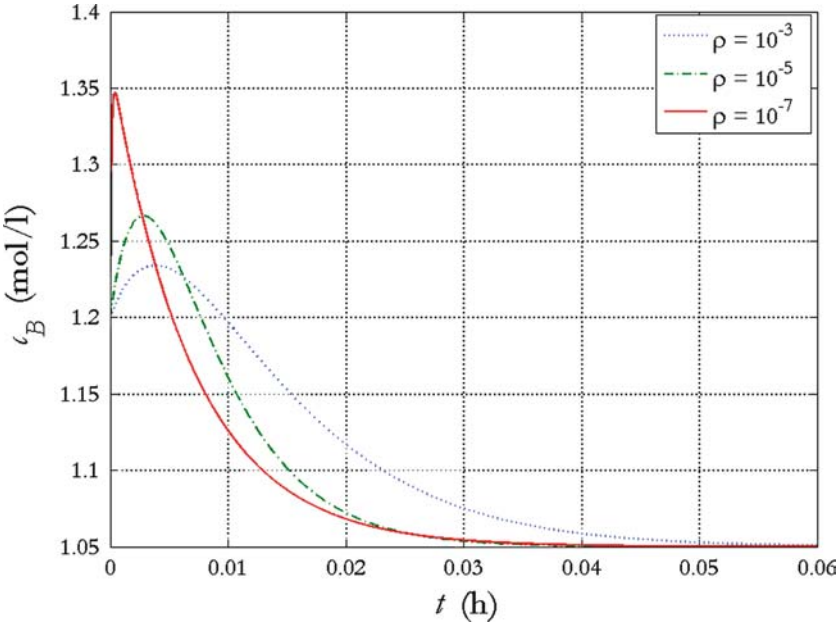

Figure 3. Optimal output responses to a step change in the set point from 1.2 to 1.05 gmol/l with different weight coefficient.

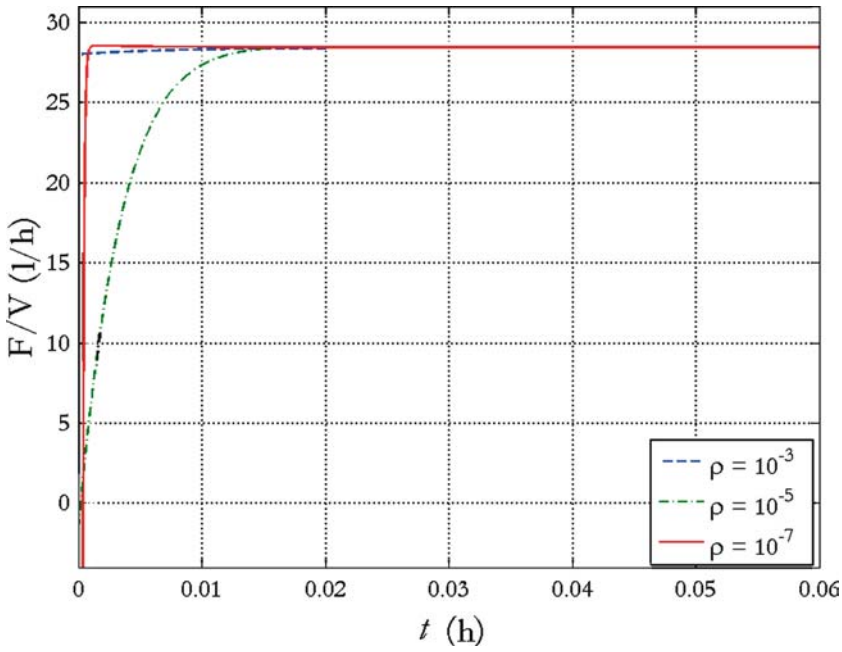

Figure 4. Optimal input responses to a step change in the set point from 1.2 to 1.05 gmol/l with different weight coefficient.

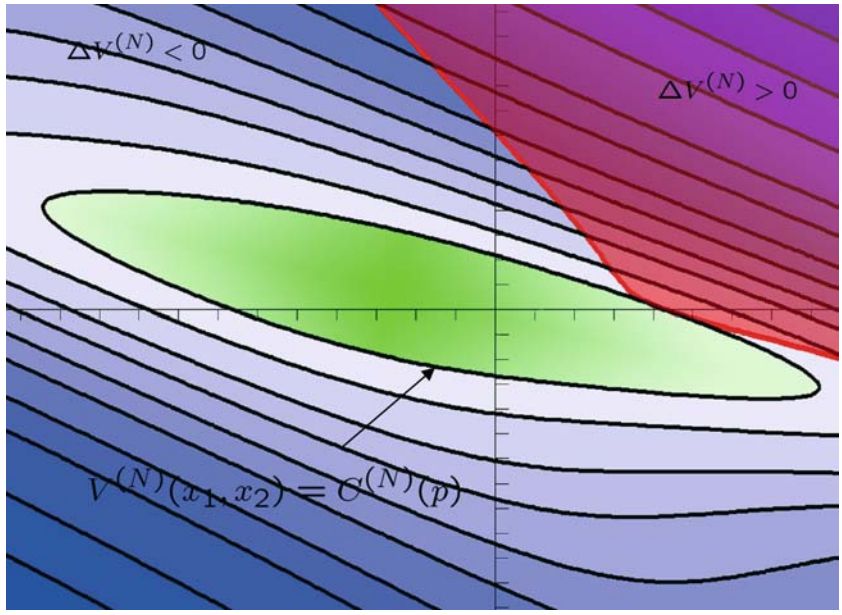

Figure 5. Geometric interpretation of the method for estimating the stability region with $N = 4$, $p_1 = 46.4$ l/h gmol, $p_2 = 57.3$ l/h gmol.

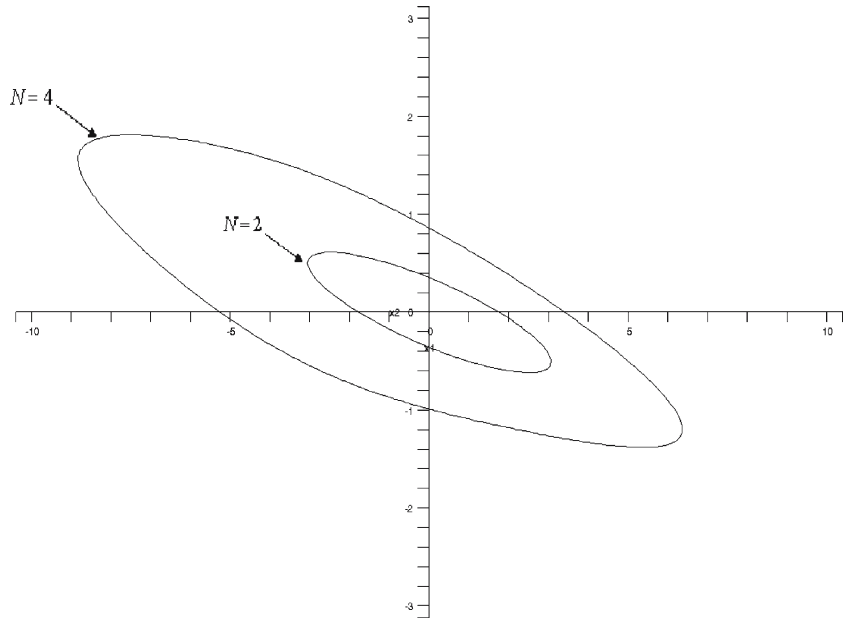

Figure 6. Stability region estimates for $N=2$ and $N=4$ with $p_1=46.4$ l/h gmol, $p_2=57.3$ l/h gmol.

5. Concluding remarks

A systematic methodology was presented that responds to the need of optimizing the digitally controlled reactor dynamics. The method is based on the explicit calculation of the value of a physically meaningful performance index through the solution of a Zubov-like functional equation. A static optimization scheme provides the optimal reactor regulator parameters, through the minimization of the parameterized performance index. The properties of the solution of the Zubov-like functional equation allow the derivation of stability region estimates associated with the controlled reactor dynamics. Finally, the proposed method was illustrated in a nonlinear chemical reactor example and its satisfactory performance demonstrated via simulation studies.

Appendix: MAPLE Code

```
> restart:
> libname:="D:/archives/maple/nlp", libname:
> readlib(mtaylor):
> readlib(coeftayl):
> with( LinearAlgebra):
```

```
> with( linalg ):
> with ( NonlinearProgramming ):
> T:=0.000001:x10:=0:x20:=0:xa0:=10:xas:=2.697:xbs:=1.05:
  fv:=28.423:k1:=50:k2:=100:k3:=10:
> Q:=x2^2+1E-5*(-p1*x1-p2*x2)^2:F1:=x1+((-x1*p1- x2*p2)*
        (xa0-xas-x1)-(fv+k1+2*k3*xas)*x1-k3*x1^2)*T:
> F2:=x2+((x1*p1+x2*p2)*(xbs+x2)+k1*x1-(k2+fv)*x2)*T:
> N:=7:
> s:=mtaylor(V(x1,x2)-V(x10,x20)-D[1](V)(x10,x20)*x1-
  D[2](V)(x10,x20)*x2,[x1=x10,x2=x20],N):
> sp:=subs([x1=F1,x2=F2],s):d:=:q(1):=:
> for j from 2 to N-1 do
    for i from 0 to j do
        p[i,j-i]:=(i!*(j-i)!)*coeftayl(s,[x1,x2]=[x10,x20],[i,j-i]):
        q(j):=q(j-1) union p[i,j-i]:
        d:=d union q(j):
    od:
  od:
> pde:=mtaylor(sp-s+Q,[x1=x10,x2=x20],N):c:=: r(1):= :
> for j from 2 to N-1 do
    for i from 0 to j do
        t[i,j-i]:=coeftayl(pde,[x1,x2]=[x10,x20],[i,j-i]):
        r(j):= r(j-1) union t[i,j-i]:
        c:=c union r(j):
    od:
  od:
> fin:=solve(c,d):
> fin:
> sol:=subs(fin,s):
> obj:=subs([x1=-0.877307434,x2=-0.16], sol):
> fun:=algsubs(p2=x[2], algsubs(p1=x[1],obj)):
> infolevel ['UnconstrainedNewton'] :=2:
> infolevel ['Optimize'] :=2:
> infolevel ['PrimalDualLogBarrier'] :=2:
> numDecVars:=2:
> x_start:=< 50, 80 >:
> UnconstrainedNewton( fun, numDecVars, x_start, 'convex', 'float[8]';
```

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