Nonlinear Controller Design via Approximate Solution of Hamilton-Jacobi Equations

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***Abstract*—This work develops a numerical algorithm for the calculation of an optimal nonlinear state feedback law for nonlinear systems. A quadratic performance index is used which contains quadratic error terms, and quadratic input penalty terms. The optimization problem is solved using the Hamilton-Jacobi equations, which determine the optimal nonlinear state feedback law. A Newton-Kantorovich iteration is developed for the solution of the pertinent Hamilton-Jacobi equations, which involves solving a Zubov partial differential equation, at each step of the iteration, using a power series method. At step N of the iteration, the method generates the (N+1)-th order truncation of the Taylor series expansion of the optimal state feedback function. The method is also applied to the problem of ISE-optimal nonminimum-phase compensation for nonlinear systems. Finally, the results are applied to the problem of controlling a nonisothermal continuous stirred tank reactor with van de Vusse kinetics.**

I. Introduction

THE Hamilton-Jacobi equation plays a central role in the theory of optimal control [7]. In the pioneer work of Al'Brekht [1] and Lukes [8], the Hamilton-Jacobi equation has been studied as the means for generating a state feedback law, which is optimal with respect to a quadratic performance index over an infinite time horizon. A power series solution approach has been formulated to generate the positive-definite solution to the Hamilton-Jacobi PDE, which could potentially be used to compute the optimal state feedback law. A variant of the Hamilton-Jacobi equation arises in nonlinear H_∞ control [10] and has been studied in a similar spirit.

There have been some engineering applications of optimal state feedback designed through the Hamilton-Jacobi equation, the most notable one being the work of Garrard and Jordan [3] in aircraft control. The key difficulty that prevented the widespread use of the Hamilton-Jacobi equation as a design tool has been the enormous computational effort and complexity in implementing Lukes' method. However, with the explosive increase in computing power in recent years, along with the availability of user-friendly and powerful symbolic computation software such as MAPLE, it is now becoming realistic to use the Hamilton-Jacobi equation as a design tool for nonlinear control applications.

The purpose of this paper is to explore the use of the Hamilton-Jacobi equation as a design tool in control problems where performance can be adequately measured via a quadratic performance index over an infinite time horizon. In order to reduce computational effort and complexity in the numerical calculations, the proposed methodology involves the application of the Newton-Kantorovich iteration to the pertinent nonlinear equations. The Newton-Kantorovich iteration as a method for solving Hamilton-Jacobi equations was first proposed and studied in a recent paper of the authors [9], for the special case of nonlinear systems that are affine in the input. The purpose of the present paper is to extend the method and results of [9] for the general case of nonlinear systems with non-affine dependence on the input. In addition, the method and results will be applied to the problem of ISE-optimal nonminimum-phase compensation for nonlinear systems.

Section II will give the problem definition and a brief review of the Hamilton-Jacobi equations for the problem under consideration. Section III will develop the Newton-Kantorovich iteration algorithm. Section IV will formulate the Hamilton-Jacobi equations for the calculation of the ISE-optimal synthetic output for nonminimum-phase nonlinear systems in normal form, and develop a Newton-Kantorovich iteration algorithm for their solution. In Section V, the results of the previous sections will be applied, tested and evaluated for a problem of regulating concentration in a nonisothermal CSTR with van de Vusse kinetics.

II. BACKGROUND

Consider a nonlinear system of the form:

$$\begin{aligned} \dot{x} &= F(x,u) \\ y &= h(x) \end{aligned} \tag{1}$$

where $x \in \mathbb{R}^n$ is the state vector, $u \in \mathbb{R}^m$ is the manipulated input vector, $y \in \mathbb{R}^m$ is the output vector, $F:\mathbb{R}^n \to \mathbb{R}^n$, and $h:\mathbb{R}^n \to \mathbb{R}^m$ are analytic functions. Without loss of generality, it can be assumed that the origin $x_0 = 0$ is an equilibrium point for system (1) corresponding to $u_0 = 0$.

Let's consider now the following quadratic performance index:

$$J = \int_0^\infty \sum_{i=1}^m \left\{ q_i \left[h_i(x) \right]^2 + r_i \left[u_i \right]^2 \right\} dt \tag{2}$$

where $h_1(x), h_2(x), \ldots, h_m(x)$ are the components of the output map $h(x)$ and $u_1, u_2, \ldots, u_m$ are the components of the input vector u, or equivalently

$$\begin{aligned} J &= \int_0^\infty \left\{ \left[h(x) \right]^T Q \left[h(x) \right] + u^T R u \right\} dt = \\ &= \int_0^\infty L(x,u)\, dt \end{aligned} \tag{3}$$

where $Q = \text{diag}\{q_1, q_2, \ldots, q_m\}$ and $R = \text{diag}\{r_1, r_2, \ldots, r_m\}$. The performance index contains quadratic error terms for output regulation with weight coefficients q_i, and quadratic input penalty terms with weight coefficients r_i.

The optimal control problem involves the minimization of the performance index (3) subject to the dynamics (1). The Hamiltonian function associated with this problem is [2]:

$$\begin{aligned} H(x,u,\lambda) &= L(x,u) + \lambda^T F(x,u) = \\ &= \left[h(x) \right]^T Q \left[h(x) \right] + u^T R u + \lambda^T F(x,u) \end{aligned}$$
(4)

where $\lambda \in \mathbb{R}^n$ is the vector of multipliers, and the corresponding Hamilton – Jacobi equation is [7]:

$$L\left(x, u^*(x)\right) + \frac{\partial V}{\partial x}(x) F\left(x, u^*(x)\right) = 0 \tag{5}$$

where

$$\begin{aligned} u^*(x) &= \arg\min_u \left\{ L(x,u) + \frac{\partial V}{\partial x}(x) F(x,u) \right\} = \\ &= \arg\min_u \left\{ \left[h(x) \right]^T Q \left[h(x) \right] + u^T R u + \frac{\partial V}{\partial x}(x) F(x,u) \right\} \end{aligned} \tag{6}$$

Consequently, the functions $V(x)$ and $u^*(x)$ must satisfy the equations:

$$\frac{\partial V}{\partial x}(x) F\left(x, u^*(x)\right) + \left[h(x) \right]^T Q \left[h(x) \right] + \left[u^*(x) \right]^T R \left[u^*(x) \right] = 0 \tag{7}$$

and

$$\frac{\partial V}{\partial x}(x)\frac{\partial F}{\partial u}\left(x,u^*(x)\right)+2\left[u^*(x)\right]^T R=0 \tag{8}$$

The optimal feedback law $u=u^*(x)$ is computed by solving the above equations with respect to $V(x)$, and $u^*(x)$.

Assuming that the system (1) is linearly controllable:

$$Rank\begin{bmatrix}\frac{\partial F}{\partial u}(0) & \frac{\partial F}{\partial x}(0)\frac{\partial F}{\partial u}(0) & \ldots & \left[\frac{\partial F}{\partial x}(0)\right]^{n-1}\frac{\partial F}{\partial u}(0)\end{bmatrix}=n$$

and linearly observable:

$$Rank\begin{bmatrix}\frac{\partial h}{\partial x}(0)\\ \frac{\partial h}{\partial x}(0)\frac{\partial F}{\partial x}(0)\\ \vdots\\ \frac{\partial h}{\partial x}(0)\left[\frac{\partial F}{\partial x}(0)\right]^{n-1}\end{bmatrix}=n$$

(7) and (8) admit a unique locally positive definite solution $V(x)$, which is locally analytic around the origin [8].

III. NEWTON- KANTOROVICH ITERATION AND ITS APPLICATION TO THE HAMILTON-JACOBI EQUATION

The Newton-Kantorovich iteration [4] is a generalization of the Newton-Raphson iteration, which is commonly used for the numerical solution of nonlinear algebraic equations, to general nonlinear operator equations $\mathcal{N}(\upsilon)=0$, where the operator $\mathcal{N}$ maps a Banach space to another. At the N-th step of the Newton-Kantorovich iteration, the following linear operator equation is solved for υ_{N+1}:

$$\mathcal{N}'(\upsilon_N)\cdot(\upsilon_{N+1}-\upsilon_N)=-\mathcal{N}(\upsilon_N) \tag{9}$$

where υ_N is the result of the (N–1)-th step and $\mathcal{N}'(\upsilon)\cdot\delta\upsilon$ is the Fréchet differential of the operator $\mathcal{N}$.

The nonlinear operator of the Hamilton-Jacobi equations (7) and (8), is:

$$\mathcal{N}(V,u^*)=\begin{bmatrix}\frac{\partial V}{\partial x}F\left(x,u^*\right)+\left[h(x)\right]^T Q\left[h(x)\right]+u^{*T}Ru^*\\ \frac{\partial V}{\partial x}\frac{\partial F}{\partial u}\left(x,u^*\right)+2u^{*T}R\end{bmatrix} \tag{10}$$

and its Fréchet differential is:

$$\mathcal{N}'(V,u^*)\cdot\begin{bmatrix}\delta V\\ \delta u^*\end{bmatrix}=\begin{bmatrix}\dfrac{\partial(\delta V)}{\partial x}F\left(x,u^*\right)+\left\{\dfrac{\partial V}{\partial x}\dfrac{\partial F}{\partial u}\left(x,u^*\right)+2u^{*T}R\right\}\delta u^*\\ \dfrac{\partial(\delta V)}{\partial x}\dfrac{\partial F}{\partial u}\left(x,u^*\right)+\delta u^{*T}\left\{\left[\dfrac{\partial^2}{\partial u^2}\left(\dfrac{\partial V}{\partial x}F\left(x,u\right)\right)\right]_{u=u^*}+2R\right\}\end{bmatrix}$$

Therefore, the Newton – Kantorovich Iteration involves solving the following linear equations, at each step of the iteration:

$$\frac{\partial\left(V_{N+1}-V_N\right)}{\partial x}F\left(x,u_N^*\right)+\left\{\frac{\partial V_N}{\partial x}\frac{\partial F}{\partial u}\left(x,u_N^*\right)+2u_N^{*T}R\right\}\left(u_{N+1}^*-u_N^*\right)=-\left\{\frac{\partial V_N}{\partial x}F\left(x,u_N^*\right)+\left[h\left(x\right)\right]^TQ\left[h\left(x\right)\right]+u_N^{*T}Ru_N^*\right\}\qquad(11)$$

and

$$\frac{\partial\left(V_{N+1}-V_N\right)}{\partial x}\frac{\partial F}{\partial u}\left(x,u_N^*\right)+\left(u_{N+1}^*-u_N^*\right)^T\left\{\left[\frac{\partial^2}{\partial u^2}\left(\frac{\partial V_N}{\partial x}F\left(x,u\right)\right)\right]_{u=u_N^*}+2R\right\}=-\left\{\frac{\partial V_N}{\partial x}\frac{\partial F}{\partial u}\left(x,u_N^*\right)+2u_N^{*T}R\right\}\qquad(12)$$

Equation (12) is a linear algebraic equation in $\left(u_{N+1}^*-u_N^*\right)$ which is readily solvable, as long as $\left[\left[\frac{\partial^2}{\partial u^2}\left(\frac{\partial V_N}{\partial x}F\left(x,u\right)\right)\right]_{u=u_N^*}+2R\right]$ is an invertible matrix. Substituting the result to (11), equations (11) and (12) can be written equivalently as

$$\begin{aligned}&\frac{\partial V_{N+1}}{\partial x}\left\{F\left(x,u_N^*\right)-\frac{\partial F}{\partial u}\left(x,u_N^*\right)\left[\left[\frac{\partial^2}{\partial u^2}\left(\frac{\partial V_N}{\partial x}F\left(x,u\right)\right)\right]_{u=u_N^*}+2R\right]^{-1}\left(\left[\frac{\partial F}{\partial u}\left(x,u_N^*\right)\right]^T\left[\frac{\partial V_N}{\partial x}\right]^T+2Ru_N^*\right)\right\}\\&=-\left\{\left[h\left(x\right)\right]^TQ\left[h\left(x\right)\right]+u_N^{*T}Ru_N^*-2u_N^{*T}R\left[\left[\frac{\partial^2}{\partial u^2}\left(\frac{\partial V_N}{\partial x}F\left(x,u\right)\right)\right]_{u=u_N^*}+2R\right]^{-1}\left(\left[\frac{\partial F}{\partial u}\left(x,u_N^*\right)\right]^T\left[\frac{\partial V_N}{\partial x}\right]^T+2Ru_N^*\right)\right\}\end{aligned}\qquad(13)$$

and

$$u_{N+1}^*=u_N^*-\left[\left[\frac{\partial^2}{\partial u^2}\left(\frac{\partial V_N}{\partial x}F\left(x,u\right)\right)\right]_{u=u_N^*}+2R\right]^{-1}\left(\left[\frac{\partial F}{\partial u}\left(x,u_N^*\right)\right]^T\left[\frac{\partial V_{N+1}}{\partial x}\right]^T+2Ru_N^*\right)\qquad(14)$$

Notice that (13) is a Zubov equation of the form

$$\frac{\partial V_{N+1}}{\partial x}(x)F_N(x)=-Q_N(x)\qquad(15)$$

where

$$F_N(x)=F\left(x,u_N^*\right)-\frac{\partial F}{\partial u}\left(x,u_N^*\right)\left[\left[\frac{\partial^2}{\partial u^2}\left(\frac{\partial V_N}{\partial x}F\left(x,u\right)\right)\right]_{u=u_N^*}+2R\right]^{-1}\left(\left[\frac{\partial F}{\partial u}\left(x,u_N^*\right)\right]^T\left[\frac{\partial V_N}{\partial x}\right]^T+2Ru_N^*\right)$$

$$Q_N(x) = \left[h(x)\right]^T Q\left[h(x)\right] + u_N^{*T} R u_N^* - 2u_N^{*T} R \left[\left[\frac{\partial^2}{\partial u^2}\left(\frac{\partial V_N}{\partial x} F(x,u)\right)\right]_{u=u_N^*} + 2R\right]^{-1} \left(\left[\frac{\partial F}{\partial u}\left(x, u_N^*\right)\right]^T \left[\frac{\partial V_N}{\partial x}\right]^T + 2Ru_N^*\right)$$

The Zubov equation (15) is a singular partial differential equation for which a recursive power series solution algorithm is applicable [5]. Once the Zubov equation is solved for $V_{N+1}(x)$, the function $u_{N+1}^*(x)$ can be immediately obtained from (14).

When the Hamilton-Jacobi equations of the previous section are applied to the linear approximation of system (1), the leading terms of the Taylor series expansion of $V(x)$, and $u^*(x)$ (quadratic and linear terms, respectively) are obtained:

$$V_1(x) = x^T P x \tag{16}$$

and

$$u_1^*(x) = -R^{-1}\left[\frac{\partial F}{\partial u}(0)\right]^T Px \tag{17}$$

where P is the positive definite solution of the algebraic Riccati equation:

$$\begin{aligned} &\left[\frac{\partial F}{\partial x}(0)\right]^T P + P\left[\frac{\partial F}{\partial x}(0)\right] - \\ -P&\left[\frac{\partial F}{\partial u}(0)\right] R^{-1} \left[\frac{\partial F}{\partial u}(0)\right]^T P + \left[\frac{\partial h}{\partial x}(0)\right]^T Q\left[\frac{\partial h}{\partial x}(0)\right] = 0 \end{aligned} \tag{18}$$

The above approximations for $V(x)$, and $u^*(x)$ are convenient initial conditions for the Newton – Kantorovich iteration of (13) and (14). In this way, the algorithm starts with the exact quadratic terms of $V(x)$ and the exact linear terms in $u^*(x)$, the task being to iteratively determine the coefficients of the higher-order terms. Moreover, it is meaningful to progressively increase the truncation order for the approximate solution of the Zubov equation from iteration to iteration, i.e calculate $V_2(x)$ up to third order, $V_3(x)$ up to fourth order, … , $V_{N+1}(x)$ up to order (N+2), and the corresponding $u_{N+1}^*(x)$ up to order (N+1). This truncation pattern was found to be most effective from a computational point of view and was followed in the numerical calculations of the Example section.

IV. ISE-OPTIMAL NONMINIMUM-PHASE COMPENSATION

Consider a SISO nonlinear system, with input u and output y, and a normal-form description of its dynamics

$$\begin{aligned} \dot{\zeta}_1 &= F_1(\zeta_1, \ldots, \zeta_{n-r}, y) \\ &\vdots \\ \dot{\zeta}_{n-r} &= F_{n-r}(\zeta_1, \ldots, \zeta_{n-r}, y) \\ \dot{y} &= y^{[1]} \\ &\vdots \\ \dot{y}^{[r-2]} &= y^{[r-1]} \\ \dot{y}^{[r-1]} &= F_y(\zeta_1, \ldots, \zeta_{n-r}, y, y^{[1]}, \ldots, y^{[r-1]}) + G(\zeta_1, \ldots, \zeta_{n-r}, y, y^{[1]}, \ldots, y^{[r-1]})\, u \end{aligned} \tag{19}$$

where r is the relative order of the system. Assume that the system is nonminimum-phase i.e its zero dynamics

$$\begin{aligned}\dot{\zeta}_1 &= F_1(\zeta_1,\ldots,\zeta_{n-r},\upsilon)\\ &\vdots\\ \dot{\zeta}_{n-r} &= F_{n-r}(\zeta_1,\ldots,\zeta_{n-r},\upsilon)\end{aligned} \tag{20}$$

where υ a reference value for the output, is unstable. Also, consider the problem of optimal regulation of the output y to a constant set point value υ, in the sense of minimizing the Integral of the Square of the Error (ISE):

$$ISE = \frac{1}{2}\int_0^\infty \left[\upsilon - y(t)\right]^2 dt \tag{21}$$

Minimisation of the performance index (21) is to be performed subject to the dynamics (19) and closed-loop stability. This is a singular optimal control problem, since, as can be easily verified, its Hamiltonian function is linear in the input u [2]. However, minimization of (21) subject to the first $(n-r)$ equations of (19) and closed-loop stability is a regular optimal control problem:

$$\boxed{\begin{array}{c}\min \quad ISE = \frac{1}{2}\int_0^\infty \left[\upsilon - y(t)\right]^2 dt\\ \text{subject to the dynamics}\\ \dot{\zeta} = F_0(\zeta, y)\\ \text{and closed-loop stability}\end{array}} \tag{22}$$

where $\zeta = \begin{bmatrix}\zeta_1\\ \vdots\\ \zeta_{n-r}\end{bmatrix}$ and $F_0(\zeta,y) = \begin{bmatrix}F_1(\zeta,y)\\ \vdots\\ F_{n-r}(\zeta,y)\end{bmatrix}$.

When the solution to the optimal control problem (22) is expressed in the form of state feedback law

$$y = y^*(\zeta;\upsilon) \tag{23}$$

this represents exactly the singular surface for the original singular optimal control problem. Note that, by construction, the function y^* will be such that the dynamics $\dot{\zeta} = F_0\left(\zeta, y^*(\zeta;\upsilon)\right)$ is stable and $y^*(\zeta_s;\upsilon) = \upsilon$.
Moreover, solving (23) with respect to υ,

$$\upsilon = h'(\zeta, y) \tag{24}$$

this defines an auxiliary output map

$$y' = h'(\zeta, y) \tag{25}$$

that possesses the following properties:

i) $h'(\zeta_s,\upsilon) = \upsilon$, which implies that y' is statically equivalent to y.

ii) the zero dynamics of system (19) with output (25) is $\dot{\zeta} = F_0\left(\zeta, y^*(\zeta;\upsilon)\right)$, which is stable, therefore y' is a minimum-phase output.

iii) Since the ISE–optimal trajectories for $\zeta(t)$ and $y(t)$ will satisfy (23) for every t, this means they will also satisfy $h'\left(\zeta(t), y(t)\right) = \upsilon$ for every t, i.e. they will correspond to perfect control of y' to υ.

Consequently, $y' = h'(\zeta, y)$ is the ISE–optimal choice of statically equivalent minimum–phase output in the sense that its perfect control to set point corresponds to ISE–optimality in the original output [11].

In what follows, a Hamilton-Jacobi formulation and solution method for the optimal control problem (22) will be developed, under the following standing assumptions:

(A1) $\frac{\partial F_0}{\partial \zeta}(\zeta_s, \upsilon)$ does not have any eigenvalues on the imaginary axis

(A2) $\left(\frac{\partial F_0}{\partial \zeta}(\zeta_s, \upsilon), \frac{\partial F_0}{\partial y}(\zeta_s, \upsilon)\right)$ form a controllable pair

where ζ_s is the equilibrium value of ζ corresponding to $y = \upsilon$.

The Hamiltonian function associated with this problem is [2]:

$$H(\zeta, y, \lambda) = \frac{1}{2}(\upsilon - y)^2 + \lambda^{\mathrm{T}} F_0(\zeta, y) \tag{26}$$

where $\lambda \in \mathbb{R}^{n-r}$ is the vector of multipliers.

Denoting

$$\kappa(\zeta, \lambda) = \arg\min_y H(\zeta, y, \lambda) \tag{27}$$

the Hamilton–Jacobi equation is [7]:

$$\frac{1}{2}\left(\upsilon - \kappa\left(\zeta, \frac{\partial V}{\partial \zeta}(\zeta)\right)\right)^2 + \frac{\partial V}{\partial \zeta}(\zeta) F_0\left(\zeta, \kappa\left(\zeta, \frac{\partial V}{\partial \zeta}(\zeta)\right)\right) = 0 \tag{28}$$

and the optimal control can be derived from the solution to the above equation, as:

$$y^* = \kappa\left(\zeta, \frac{\partial V}{\partial \zeta}(\zeta)\right) \tag{29}$$

Equivalently, since $\frac{\partial H}{\partial y}(\zeta, y, \lambda)$ must vanish at $\arg\min_y H(\zeta, y, \lambda)$, the functions $V(\zeta)$ and $y^*(\zeta)$ must satisfy the coupled equations:

$$\boxed{\begin{array}{c} \frac{1}{2}\left(\upsilon - y^*(\zeta)\right)^2 + \frac{\partial V}{\partial \zeta}(\zeta) F_0\left(\zeta, y^*(\zeta)\right) = 0 \\ \upsilon - y^*(\zeta) - \frac{\partial V}{\partial \zeta}(\zeta) \frac{\partial F_0}{\partial y}\left(\zeta, y^*(\zeta)\right) = 0 \end{array}} \tag{30}$$

The above equations must be solved with initial conditions:

$$\boxed{V(\zeta_s) = 0 \quad , \quad y^*(\zeta_s) = \upsilon} \tag{31}$$

Under the assumption of analyticity of $F_0 : \mathbb{R}^{n-r} \times \mathbb{R} \to \mathbb{R}^{n-r}$, together with assumptions (A1) and (A2) stated in the previous section, there exists a unique analytic solution in a neighbourhood of $\zeta = \zeta_s$, such that the dynamics $\dot{\zeta} = F_0\left(\zeta, y^*(\zeta)\right)$ is locally asymptotically stable [8]. The solution for $V(\zeta)$ is locally positive semidefinite.

Given the local analyticity property of the solution, it is possible to seek for the solution in the form of a Taylor series expansion and, recursively try to determine the Taylor coefficients up to a certain truncation order [8]. When this approach is applied to the leading terms of the Taylor series expansion (quadratic terms in $V(\zeta)$ and linear terms in $y^*(\zeta)$), one obtains the solution for the linear–quadratic approximation of the problem:

$$V(\zeta)=\frac{1}{2}(\zeta-\zeta_s)^{\mathrm{T}}P(\zeta-\zeta_s)+O(\zeta^3) \tag{32}$$

$$y^*(\zeta)=\upsilon-\left[\frac{\partial F_0}{\partial y}(\zeta_s,\upsilon)\right]^{\mathrm{T}}P(\zeta-\zeta_s)+O(\zeta^2) \tag{33}$$

where P is the solution of the quadratic matrix equation:

$$\left[\frac{\partial F_0}{\partial \zeta}(\zeta_s,\upsilon)\right]^{\mathrm{T}}P+P\left[\frac{\partial F_0}{\partial \zeta}(\zeta_s,\upsilon)\right]-P\left[\frac{\partial F_0}{\partial y}(\zeta_s,\upsilon)\right]\left[\frac{\partial F_0}{\partial y}(\zeta_s,\upsilon)\right]^{\mathrm{T}}P=0 \tag{34}$$

that makes $\left[\frac{\partial F_0}{\partial \zeta}(\zeta_s,\upsilon)\right]-\left[\frac{\partial F_0}{\partial y}(\zeta_s,\upsilon)\right]\left[\frac{\partial F_0}{\partial y}(\zeta_s,\upsilon)\right]^{\mathrm{T}}P$ Hurwitz.

The procedure can, in principle, continue, to determine the coefficients of the higher-order terms of the Taylor series expansion of the solution, but the resulting algebraic equations are nonlinear and extremely complex. However, as in the previous section, the solution of the Hamilton-Jacobi equations (30) can be facilitated by applying the Newton-Kantorovich iteration.

In particular, for the nonlinear operator $\mathcal{N}(V,y^*)=\begin{bmatrix}\frac{1}{2}(\upsilon-y^*)^2+\frac{\partial V}{\partial\zeta}F_0(\zeta,y^*)\\ -(\upsilon-y^*)+\frac{\partial V}{\partial\zeta}\frac{\partial F_0}{\partial y}(\zeta,y^*)\end{bmatrix}$, the Fréchet differential is:

$$\mathcal{N}'(V,y^*)\cdot\begin{bmatrix}\delta V\\ \delta y^*\end{bmatrix}=\begin{bmatrix}\frac{\partial(\delta V)}{\partial\zeta}F_0(\zeta,y^*)+\left(y^*-\upsilon+\frac{\partial V}{\partial\zeta}\frac{\partial F_0}{\partial y}(\zeta,y^*)\right)\delta y^*\\ \frac{\partial(\delta V)}{\partial\zeta}\frac{\partial F_0}{\partial y}(\zeta,y^*)+\left(1+\frac{\partial V}{\partial\zeta}\frac{\partial^2 F_0}{\partial y^2}(\zeta,y^*)\right)\delta y^*\end{bmatrix} \tag{35}$$

and therefore, the Newton-Kantorovich iteration involves solving the following linear equations at each step of the iteration:

$$\frac{\partial(V_{N+1}-V_N)}{\partial\zeta}F_0(\zeta,y_N^*)+\left(y_N^*-\upsilon+\frac{\partial V_N}{\partial\zeta}\frac{\partial F_0}{\partial y}(\zeta,y_N^*)\right)(y_{N+1}^*-y_N^*)=-\frac{1}{2}(\upsilon-y_N^*)^2-\frac{\partial V_N}{\partial\zeta}F_0(\zeta,y_N^*) \tag{36}$$

$$\frac{\partial(V_{N+1}-V_N)}{\partial\zeta}\frac{\partial F_0}{\partial y}(\zeta,y_N^*)+\left(1+\frac{\partial V_N}{\partial\zeta}\frac{\partial^2 F_0}{\partial y^2}(\zeta,y_N^*)\right)(y_{N+1}^*-y_N^*)=\upsilon-y_N^*-\frac{\partial V_N}{\partial\zeta}\frac{\partial F_0}{\partial y}(\zeta,y_N^*) \tag{37}$$

Solving (37) for $(y_{N+1}^*-y_N^*)$, substituting the result into (36), rearranging and collecting terms, the Newton-Kantorovich iteration takes the form:

$$\frac{\partial V_{N+1}}{\partial\zeta}\left[F_0(\zeta,y_N^*)-\frac{\partial F_0}{\partial y}(\zeta,y_N^*)\frac{y_N^*-\upsilon+\frac{\partial V_N}{\partial\zeta}\frac{\partial F_0}{\partial y}(\zeta,y_N^*)}{1+\frac{\partial V_N}{\partial\zeta}\frac{\partial^2 F_0}{\partial y^2}(\zeta,y_N^*)}\right]+\frac{1}{2}(y_N^*-\upsilon)^2-(y_N^*-\upsilon)\frac{y_N^*-\upsilon+\frac{\partial V_N}{\partial\zeta}\frac{\partial F_0}{\partial y}(\zeta,y_N^*)}{1+\frac{\partial V_N}{\partial\zeta}\frac{\partial^2 F_0}{\partial y^2}(\zeta,y_N^*)}=0 \tag{38}$$

$$y_{N+1}^{*}=y_{N}^{*}-\frac{y_{N}^{*}-\upsilon+\dfrac{\partial V_{N+1}}{\partial\zeta}\dfrac{\partial F_{0}}{\partial y}\left(\zeta,y_{N}^{*}\right)}{1+\dfrac{\partial V_{N}}{\partial\zeta}\dfrac{\partial^{2}F_{0}}{\partial y^{2}}\left(\zeta,y_{N}^{*}\right)} \tag{39}$$

Equation (38) is a Zubov partial differential equation with unknown $V_{N+1}(\zeta)$, which can be solved using the recursive series solution algorithm of [5]. Once the solution of (38) is computed, (39) determines directly $y_{N+1}^{*}(\zeta)$.

The Newton–Kantorovich iteration can be initialized with $V_1(\zeta)$ quadratic and $y_1^{*}(\zeta)$ linear, obtained from the linear–quadratic approximation of the problem, given by (32) and (33), and then, progressively increasing the truncation order in the solution of the Zubov equation for $V_{N+1}(\zeta)$ and the corresponding $y_{N+1}^{*}(\zeta)$.

V. EXAMPLE

Consider a nonisothermal continuous stirred tank reactor (CSTR) of constant volume V, in which the following series/parallel reaction takes place:

$$A\xrightarrow{k_1}B\xrightarrow{k_2}C$$
$$2A\xrightarrow{k_3}D$$

The mass and energy balances that describe the dynamics of the reactor are:

$$\begin{aligned}
\frac{dC_A}{dt}&=-k_1(T)C_A-k_3(T)C_A^2+\left(C_A^0-C_A\right)\frac{F}{V}\\
\frac{dC_B}{dt}&=k_1(T)C_A-k_2(T)C_B-C_B\frac{F}{V}\\
\frac{dT}{dt}&=\frac{-\left(\Delta H_1\right)k_1(T)C_A-\left(\Delta H_2\right)k_2(T)C_B-\left(\Delta H_3\right)k_3(T)C_A^2}{\rho_{mix}C_P}+\frac{Q_H}{\rho_{mix}C_P}+\left(T^0-T\right)\frac{F}{V}\\
y&=C_B
\end{aligned} \tag{40}$$

where C_A, C_B are the molar concentrations of A and B respectively, T the temperature of the reactor, $\frac{F}{V}$ the dilution rate, ρ_{mix} the density of the mixture, C_P the heat capacity, ΔH_i the heats of the reaction and Q_H the constant rate of the heat removed per unit volume. The rate coefficients are given by the Arrhenius equation $k_i(T)=k_{i0}\exp(-E_i/RT)$, $i=1,2,3$. All the constants and parameters are given in Table 1 [6].

TABLE 1
CONSTANTS AND PARAMETERS OF THE SYSTEM

$k_{10}=1.287\cdot10^{12}h^{-1}$	$k_{20}=1.287\cdot10^{12}h^{-1}$	$k_{30}=9.043\cdot10^{9}L/(mol\cdot h)$
$E_1/R=9758.3K$	$E_2/R=9758.3K$	$E_3/R=8560K$
$\Delta H_1=4.2kJ/mol$	$\Delta H_2=-11kJ/mol$	$\Delta H_3=-41.85kJ/mol$
$\rho_{mix}=0.9342kg/L$	$C_P=3.01kJ/(kg\cdot K)$	$Q_H=-451.51kJ/(L\cdot h)$
$C_A^0=5gmol/L$	$T^0=403.15K$	

The control objective is the optimal regulation of the output $y = C_B$ at set point by manipulating the dilution rate $\frac{F}{V}$. In particular, the controller must bring the system to the final steady state of $C_{As} = 1.0774\, mol/L$, $C_{Bs} = 0.8181\, mol/L$ and $T_s = 403.15 K$, which corresponds to $(F/V)_s = 12.5418\, h^{-1}$.

The system (40) has relative order $r = 1$ and can be transformed to normal form (19) via the coordinate transformation

$$\zeta_1 = \frac{C_A^0 - C_A}{C_B}, \quad \zeta_2 = \frac{T^0 - T}{C_B}, \quad y = C_B \tag{41}$$

The transformed system is:

$$\begin{aligned}
\frac{d\zeta_1}{dt} &= \kappa_1(1-\zeta_1)\frac{C_A^0 - \zeta_1 y}{y} + \kappa_2\zeta_1 + \kappa_3\frac{\left(C_A^0 - \zeta_1 y\right)^2}{y} \\
\frac{d\zeta_2}{dt} &= \kappa_1\left(\frac{\Delta H_1}{\rho_{mix}C_p} - \zeta_2\right)\frac{C_A^0 - \zeta_1 y}{y} + \kappa_2\left(\zeta_2 + \frac{\Delta H_2}{\rho_{mix}C_p}\right) + \frac{\kappa_3 \Delta H_3}{\rho_{mix}C_p}\frac{\left(C_A^0 - \zeta_1 y\right)^2}{y} - \frac{Q_H}{\rho_{mix}C_p}\frac{1}{y} \\
\frac{dy}{dt} &= \kappa_1\left(C_A^0 - \zeta_1 y\right) - \kappa_2 y - y\frac{F}{V}
\end{aligned} \tag{42}$$

where $\kappa_i = k_{i0}\exp\left\{-E_i / R(T^0 - \zeta_2 y)\right\}$, $i = 1,2,3$.
The first two equations of (42), with the output y at its reference steady-state value, represent the zero dynamics.

Coordinate transformation (41) maps the desirable final steady state to $\zeta_{1s} = 4.7948$, $\zeta_{2s} = 0$ and $y_s = 0.8181\, mol/L$. A straightforward calculation of the eigenvalues of the Jacobian of the zero dynamics shows that the system is nonminimum-phase at the desirable final steady state.

System (40) or (42) will be controlled to the desirable final steady state through two alternative methods:
a) direct calculation of the optimal state feedback by minimizing a quadratic performance index representing a combination of an error measure and a control effort measure (composite index)
b) calculation of the ISE-optimal minimum-phase output and input/output linearization on that output

a) optimal state feedback with respect to composite quadratic index

Using deviation variables:

$$x_1 = C_A - C_A^s,\; x_2 = C_B - C_B^s,\; x_3 = T - T^s \quad u = F/V - \left(F/V\right)^s$$

the system (40) is put in the form of system (1) and the objective is to compute the optimal state-feedback control law, so that the following performance index is minimized:

$$J = \int_0^\infty \left\{x_2^2 + \rho u^2\right\} dt \tag{43}$$

The Hamilton-Jacobi equations for this case (1 input, 1 output and 3 states) take the form:

$$\begin{aligned}
&\frac{\partial V}{\partial x_1}(x_1,x_2,x_3)F_1(x_1,x_2,x_3,u^*) + \frac{\partial V}{\partial x_2}(x_1,x_2,x_3)F_2(x_1,x_2,x_3,u^*) + \frac{\partial V}{\partial x_3}(x_1,x_2,x_3)F_3(x_1,x_2,x_3 u^*) \\
&\qquad + \left[h(x_1,x_2,x_3)\right]^2 + \rho\left[u^*(x_1,x_2,x_3)\right]^2 = 0
\end{aligned} \tag{44}$$

where $u^*(x_1,x_2,x_3,x_4)$ satisfies:

$$\frac{\partial V}{\partial x_1}(x_1,x_2,x_3)\frac{\partial F_1}{\partial u}(x_1,x_2,x_3,u^*) + \frac{\partial V}{\partial x_2}(x_1,x_2,x_3)\frac{\partial F_2}{\partial u}(x_1,x_2,x_3,u^*) + \frac{\partial V}{\partial x_3}(x_1,x_2,x_3)\frac{\partial F_3}{\partial u}(x_1,x_2,x_3,u^*) + 2\rho u^*(x_1,x_2,x_3) = 0$$

$$(45)$$

Equations (27) and (28) were solved using the symbolic program MAPLE, applying the Newton-Kantorovich iteration method described in the previous section, with initial conditions (16) and (17). At step N of the Newton-Kantorovich iteration, the Zubov equation (13) was solved via power series up to truncation order (N+2) and the resulting feedback function was calculated from (14) up to order (N+1). In this way, the truncation order was progressively increasing from iteration to iteration.

Table 2 contains representative times of program runs as a function of the truncation order for V, for the particular hardware profile of our computer (CPU 2.8 GHz and RAM 1 GB). For comparison, a MAPLE program was also written using Lukes' method and run on the same computer. This program could only be run for 3rd order truncation. For higher truncation orders, the program could not finish after a day of running.

TABLE 2
REPRESENTATIVE RUN TIMES

	Truncation Order for V	Time(s)
Iteration 1	3	0.7
Iteration 2	4	0.8
Iteration 3	5	2.0
Iteration 4	6	3.6
Iteration 5	7	6.4
Iteration 6	8	11.9
Iteration 7	9	23.8
Iteration 8	10	36.2

Figures 1 and 2 depict the optimal closed-loop responses of output C_B and input F/V, for a step change in the set-point from 0.885 to 0.8181 and for different truncation orders, $N = 2,3,4,5,7,10$, with input penalty weight $\rho = 10^{-3}$. It is clearly seen that the polynomial approximation converges from $4-\text{th}$ order truncation and over.

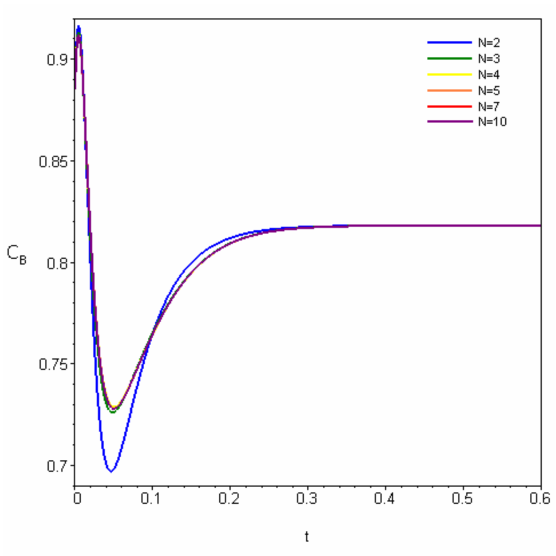

Fig. 1. Optimal output responses to a step change in the set point from 0.885 to 0.8181, for $\rho = 10^{-3}$ ($N = 2,3,4,5,7,10$)

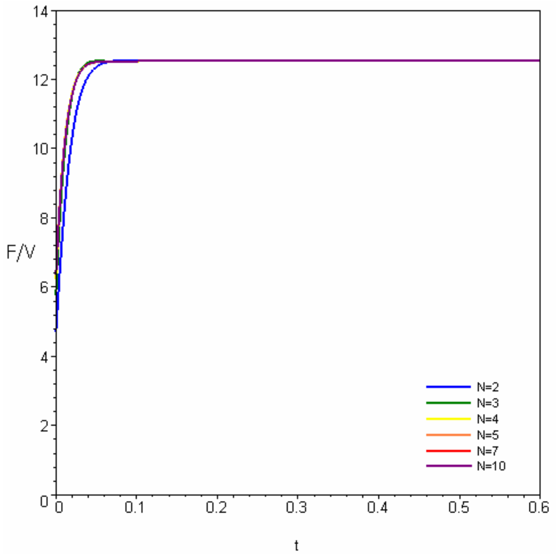

Fig. 2. Optimal input responses to a step change in the set point from 0.885 to 0.8181, for $\rho = 10^{-3}$
($N = 2,3,4,5,7,10$)

The effect of the weight coefficient ρ on the optimal closed-loop system response has also been studied. Figures 3 and 4 show the responses for the same step change in the set point and for three representative values of the weight coefficient, $\rho = 10^{-5}$, $\rho = 10^{-3}$, $\rho = 10^{-1}$. The calculations were made for $10-$th order truncation. It can be observed that small values of ρ give faster output responses but unrealistically large deviations in the dilution rate. On the other hand, large values of ρ give slower responses.

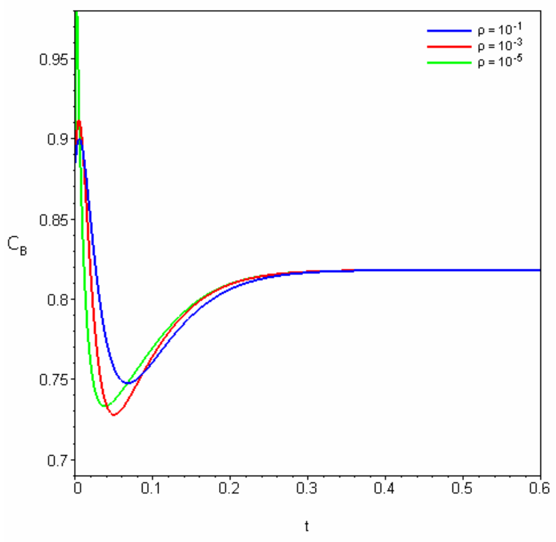

Fig. 3. Optimal output responses to a step change in the set point from 0.885 to 0.8181, for $N = 10$
($\rho = 10^{-5}$, $\rho = 10^{-3}$, $\rho = 10^{-1}$)

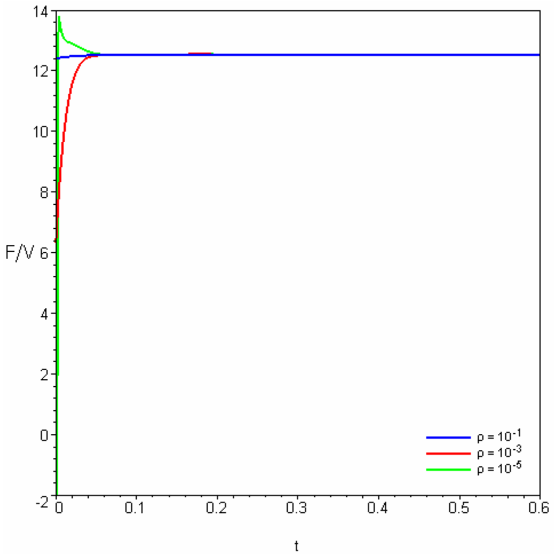

Fig. 4. Optimal input responses to a step change in the set point from 0.885 to 0.8181, for $N = 10$ ($\rho = 10^{-5}$, $\rho = 10^{-3}$, $\rho = 10^{-1}$)

b) input/output linearization on the ISE-optimal synthetic output

Using deviation variables $\bar{\zeta}_1 = \zeta_1 - \zeta_{1s}$, $\bar{\zeta}_2 = \zeta_2 - \zeta_{2s}$ and $\bar{y} = y - y_s$, the problem becomes the one of regulating the given nonminimum-phase system at the origin. In terms of deviation variables, the ISE criterion takes the form:

$$ISE = \frac{1}{2}\int_0^\infty \bar{y}^2 dt \tag{46}$$

and the Hamilton-Jacobi equations are of the form

$$\frac{1}{2}\bar{y}^{*2} + \frac{\partial V}{\partial \bar{\zeta}_1} F_1(\bar{\zeta}_1, \bar{\zeta}_2, \bar{y}^*) + \frac{\partial V}{\partial \bar{\zeta}_2} F_2(\bar{\zeta}_1, \bar{\zeta}_2, \bar{y}^*) = 0 \tag{47}$$

$$\bar{y}^* + \frac{\partial V}{\partial \bar{\zeta}_1}\frac{\partial F_1}{\partial \bar{y}}(\bar{\zeta}_1, \bar{\zeta}_2, \bar{y}^*) + \frac{\partial V}{\partial \bar{\zeta}_2}\frac{\partial F_2}{\partial \bar{y}}(\bar{\zeta}_1, \bar{\zeta}_2, \bar{y}^*) = 0 \tag{48}$$

where $F_1(\bar{\zeta}_1, \bar{\zeta}_2, \bar{y})$ and $F_2(\bar{\zeta}_1, \bar{\zeta}_2, \bar{y})$ are the right-hand sides of the first two equations of (42) in deviation variable form.

The Hamilton - Jacobi equations (47)-(48) were solved applying the Newton-Kantorovich iteration method described in the previous section. The iteration was initialized with V quadratic and y^* linear, obtained from the solution of the linear-quadratic approximation of the problem (32)-(34). At step N of the Newton-Kantorovich iteration, the Zubov equation (38) was solved using the recursive series solution algorithm of [5] up to truncation order (N+2), leading to a (N+2)-th order approximation for V and the resulting feedback function was calculated from (39) up to order (N+1). In this way, the truncation order was progressively increasing from iteration to iteration. The calculations were performed using the symbolic program MAPLE. Table 3 contains representative times of program runs as a function of the iteration number, for the particular hardware profile of our computer (CPU 2.8 GHz and RAM 1 GB).

TABLE 3
RUN TIMES FOR THE PROGRAM SOLVING THE HAMILTON-JACOBI EQUATIONS

	Time (s)
Iteration 1 (3rd order truncation for V)	9.5
Iteration 2 (4th order truncation for V)	49.5
Iteration 3 (5th order truncation for V)	1700.2

Figure 5 depicts the approximations of the solution $V_N(\bar{\zeta}_1,\bar{\zeta}_2)$ for truncation orders N=2,3,4,5. In Figure 5, the quadratic initial condition (N=2) is at the top, the result after 1 iteration (N=3) at the bottom, and the results for N=4,5 essentially coincide in the middle. This indicates that convergence has been achieved after 2 iterations within the ranges of $\bar{\zeta}_1$ and $\bar{\zeta}_2$ shown. A similar diagram was constructed for $\bar{y}^*(\bar{\zeta}_1,\bar{\zeta}_2)$ (not shown), that indicated numerical convergence after 1 iteration, within the same ranges.

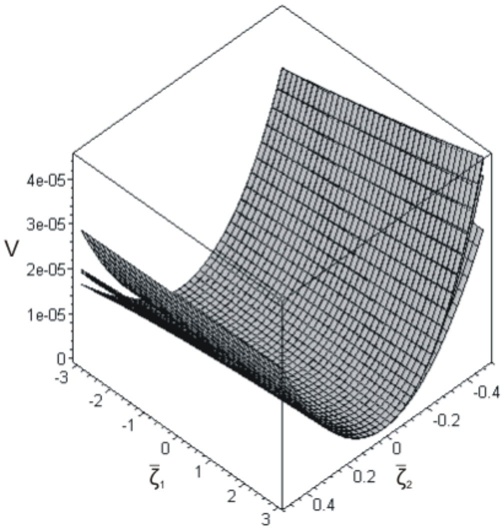

Fig. 5. Approximate solution for $V(\bar{\zeta}_1,\bar{\zeta}_2)$ for truncation orders N=2, 3, 4, 5

For nonminimum-phase compensation, the synthetic output

$$y' = \bar{y} - \bar{y}^*(\bar{\zeta}_1,\bar{\zeta}_2) \tag{49}$$

is used, which is a statically equivalent minimum-phase output and, moreover, perfect control of y' to 0 corresponds to ISE–optimality in y. An input/output linearizing state feedback law with respect to the synthetic output map (49) is then applied to regulate y' to 0.

Figures 6 and 7 show the resulting closed-loop responses of output $y = C_B$ and synthetic output y', for a step change in the set-point from 0.85 to 0.8181 and for different closed-loop time constants, $\tau=10^{-2}$, 10^{-3}, 10^{-4} and 10^{-5}. The calculations were performed using the 4-th order approximation for $\bar{y}^*$. As the closed-loop time constant τ tends to zero, the resulting closed-loop responses converge to the ISE-optimal responses.

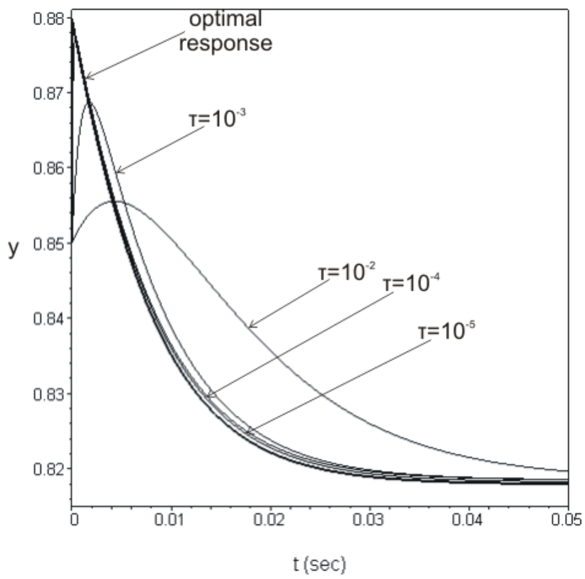

Fig. 6. Closed-loop responses of output $y = C_B$ for a step change in the set point from 0.85 to 0.8181 (τ=10^{-2}, τ=10^{-3}, τ=10^{-4}, τ=10^{-5})

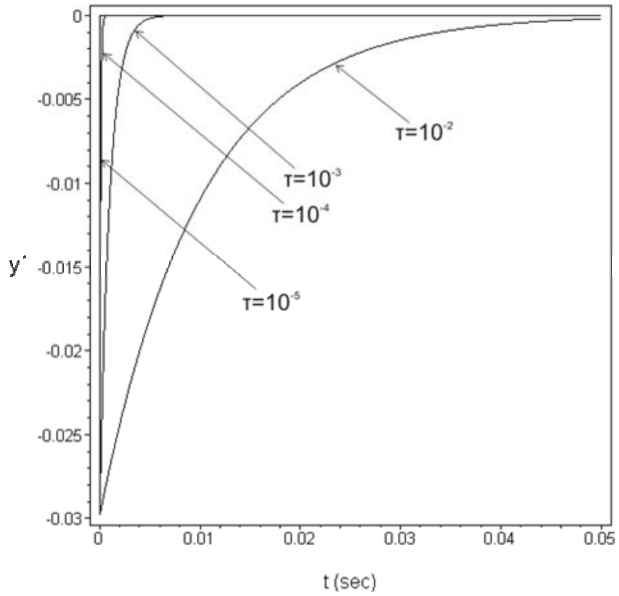

Fig. 7. Closed-loop responses of synthetic output y' for a step change in the set point from 0.85 to 0.8181 (τ=10^{-2}, τ=10^{-3}, τ=10^{-4}, τ=10^{-5})

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