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Passivity Versus Flatness in the Regulation of an Exothermic Chemical Reactor*

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We examine the performance of two nonlinear feedback trajectory tracking controllers designed to achieve the regulated transfer from a stable operating equilibrium point towards a more efficient, yet open loop unstable, equilibrium point in a nonlinear multivariable exothermic chemical reactor system. A passivity based controller, designed with reasonable passive outputs reference trajectories, is shown to be unsuitable, due to unrealistic reactant concentration and temperature controller profiles in the unrestricted controls case, or, due to controller saturation, and convergence to undesirable equilibria, when hard constraints are imposed on the control input signals. However, an exact tracking error linearization controller, designed with similar reference trajectories for the flat outputs is shown to be entirely feasible in the unrestricted controls case and, furthermore, devoid of control signals saturations in the restricted case. The differential flatness property is then used to synthesize a suitable feedback passivity based controller with passive outputs reference trajectories indirectly specified in terms of the flat output trajectories. The obtained "passivity plus flatness" (PF) controller is shown to be entirely equivalent to the "linearizing plus flatness" (LF) controller when plant parameter perturbations and initial state setting errors are absent from the equilibrium transfer maneuver. However, when such perturbations are present, the LF controller is shown to be superior to the PF controller in several respects.

Keywords: Differential flatness; Exothermic chemical reactors; Passivity

1. Introduction

Differential flatness, introduced by Prof. M. Fliess and his coworkers in [4–6], represents a remarkable structural property of systems which are linearizable by means of *endogenous* feedback. As such, it may be used to advantage in establishing the most salient features and characteristics of a given system, particularly in the context of a specific controller design technique at hand. Flatness greatly facilitates the feedback controller design task for a nonlinear multivariable system, specially, if tracking of prescribed output vector trajectories is to be enforced.

Differential flatness has been advantageously exploited in the feedback regulation of different classes of chemical reactors. The case of coupled chemical reactors was treated in an article by Rudolph [14]. Several examples of nonlinear chemical reactor control tasks were undertaken by Rothfuss et al. in [13]. The relevance of flatness in the regulation of a class

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of infinite dimensional models of chemical reactors, including time delays, was examined in an article by Mounier and Rudolph [10]. Applications of ideas related to differential flatness also include systems described by partial differential equations. In this context, an interesting application to the control of chemical reactors has been recently given in the work of Fliess et al. [7].

Passivity based control, on the other hand, also enjoys great respectability due to the relative simplicity of the control laws and the emphasis on stability by physically oriented considerations, rather than straightforward linearization. As such, passivity based controllers tend to take a clever advantage of the "dissipation structure" of the given nonlinear system by respecting those beneficial nonlinearities that help in the stabilization of the system. Typically, passivity based controllers only try to eliminate the locally destabilizing forces by means of suitable feedback. Seminal work in this area, in the context of *dissipativity*, was initiated by Willems [19]. A contribution, from a geometrical perspective, is represented by the article by Byrnes et al. [3]. Recently, a textbook by Ortega et al. [11], collects a number of specific applications, which include actual laboratory implementation, where the passivity based control design technique has been successfully used. Passivity based control of continuous chemical processes has been treated by Alonso and Ydstie in [1] from a general thermodynamics viewpoint. Recently, in an article by Sira-Ramírez and Angulo-Núñez [17], a simplified approach, based on projection operators, has been developed for the passivity based control of nonlinear systems with applications to the control of a variety of continuous processes, including bio-reactors, flow processes, and chemical reactors.

In this article, we compare the performances of a passivity based controller and an exact linearization controller in the stabilization, by means of trajectory tracking, of a particularly troublesome nonlinear exothermic chemical reactor that operates subject to hard input constraints. The reactor model used in this article has been thoroughly treated in a recent article by Viel et al. [18]. The problem consists in achieving an equilibrium transfer, from a high temperature stable operating point towards an intermediate temperature, open loop unstable, equilibrium point which is deemed desirable due to technological, and economic reasons. In [18], it is shown, for the single-input reactor model, that a controller based on straightforward partial linearization of the temperature dynamics is incapable of achieving the required equilibrium transfer due to controller saturation. This is due to the fact that the reactor cannot be sufficiently cooled off while the control input remains clamped at the lower saturation limit. As a consequence, an undesired stable equilibrium point is obtained if the partially linearizing controller is directly implemented. In [18], an alternative control input variable is then proposed which is capable of regulating the reactant concentration at the feed flow. A globally stabilizing discontinuous controller is then proposed for the new control input in combination with a "hybrid" type of controller for the customary control input signal combining the feed temperature and the coolant temperature.

By considering the exothermic reactor model as a multivariable system with two control inputs, just as proposed in [18], the resulting system is readily seen to be differentially flat, a fact not exploited in [18]. The flat outputs are the product concentration and the reactor temperature. We use the flatness property, and its associated differential parametrization, in order to exhibit the fundamental reactor system characteristics, such as the *passive* character of the reactant and product concentration variables, the *equilibrium state detectability*, as well as a static parametrization of the equilibria in terms of constant values of the flat outputs.

Using the "energy shapping plus damping injection controller design methodology", widely used in the regulation of Lagrangian mechanical and electromechanical systems (see the article by Ortega et al. [12]), we first propose a passivity based feedback controller with reasonable passive outputs reference trajectories smoothly achieving the desired equilibrium transfer. We show that this controller *does not* accomplish the required transfer due to either control input saturations or to unrealistic reactant concentration and coolant temperature profiles. We then proceed to show that an exact feedback linearization tracking error controller, based on prescribed trajectories for the flat outputs, *does* achieve the desired objective *without* input saturations. This motivates the combination of the derived passivity based controller with an indirect passive outputs reference trajectory planning in terms of the suitably planned trajectories for the systems flat outputs. The resulting "passivity plus flatness" (PF) based multivariable controller now achieves the required equilibrium transfer without inputs saturations. In fact, the PF based controller is shown to be completely equivalent to the "linearization plus flatness" (LF) controller inasmuch as the ideal, perturbation-free, tracking behaviours are concerned. However, the behaviour of both tracking controllers to initial setting errors and unmodelled plant parameter variations is significantly different. We show that the LF based controller is superior, in several respects, to the PF controller.

Section 2 briefly describes the exothermic reactor model. Section 3 derives the passivity based controller and shows the unfeasible closed loop behaviour obtained with this controller. In Section 4, a stabilizing feedback controller, based on flat outputs trajectory tracking error linearization, is presented which suitably achieves the required equilibrium transfer. In Section 5, the passivity based controller is implemented using planned passive outputs trajectories specified in terms of the flat outputs trajectories. Section 6 is devoted to some conclusions and suggestions for further research. An appendix, at the end of the article, collects the basic definitions related to flatness and passivity.

2. Description of an Exothermic Reactor

2.1. Reactor Model with Controlled Reactant Feed Concentration

Consider the following continuous multivariable reactor model, proposed in [18], in which a first order and exothermic reaction $A \rightarrow B$ occurs

$$\begin{aligned} \dot{x}_1 &= -k(x_3)x_1 + \beta(u_1 - x_1), \\ \dot{x}_2 &= k(x_3)x_1 - \beta x_2, \\ \dot{x}_3 &= \alpha k(x_3)x_1 - q x_3 + u_2, \end{aligned} \tag{2.1}$$

where x_1 is the concentration of the reactant A and x_2 is the concentration of the product B. The variable x_3 represents the reactor temperature. $\beta > 0$ is a constant associated with the dilution rate while $\alpha > 0$ is the exothermicity of the reaction. The control input u_1 represents the concentration of the reactant A in the feed flow [18]. The control input u_2 corresponds to a suitable, and well known, combination of the feed temperature T^{in} and the coolant temperature T_w. In fact, $u_2 = \beta T^{\text{in}} + \epsilon T_w$ where $\epsilon > 0$ is the heat transfer rate constant. The constant q is defined as $q = \beta + \epsilon > 0$. The function $k(x_3)$ is given by

$$k(x_3) = k_0 \exp\left(-\frac{k_1}{x_3}\right) \tag{2.2}$$

with k_0 and k_1 assumed to be known constants.

Remark 2.1. Eventhough the control input variable, u_1, may take values on a discrete set of the form $\{0, \bar{x}_1^{\text{feed}}\}$, with $\bar{x}_1^{\text{feed}}$ being the *nominal* value of the input feed concentration, our results treat u_1 as a variable *continuously* taking values on the closed restriction set, $[0, \bar{x}_1^{\text{feed}}]$. The fundamental assumption, and restriction, on u_1 is that the inlet concentration can be continuously lowered, or enhanced, by increasing or decreasing the addition of solvent. Nevertheless, input feed concentration cannot be raised above its maximum (nominal) value, denoted by $\bar{x}_1^{\text{feed}}$. An alternative justification to our approach lies in the fact that the discontinuous character ascribed in [18] to u_1 (i.e., u_1 is a *switched control input*) can be made compatible with our assumption by considering the treated model (2.1) as an *averaged* pulse-width-modulated (PWM) model of the reactor controlled dynamics. The control input u_1, under such an interpretation, qualifies as a scaled *duty ratio* control input function. In other words, u_1 is to be interpreted as the product: $\bar{x}_1^{\text{feed}}\mu_1$ with μ_1 being an *actual* duty ratio function, acting now as a truly continuous control input taking values on the closed subset [0, 1] of the real line. The synthesized duty ratio may then be implemented on a PWM feedback control scheme. Such an implementation does not necessarily demand an unrealistic, bang bang behaviour on the input feed valve. The reader is referred to [15,16], for details on dynamically smoothed PWM controller design for nonlinear systems whose exposition would take us quite far from our main purpose in this paper. □

2.2. Differential Flatness of the Multivariable Reactor Model

The multivariable controlled system (2.1) and (2.2) is easily seen to be differentially flat, with flat outputs $y = (F, M)$ given by $F = x_2$ and $M = x_3$. Indeed, the system state variables, x_1, x_2, x_3 and the control inputs u_1, u_2 are expressible as *differential functions* of the two differentially independent components of y

$$\begin{aligned} x_1 &= \frac{\dot{F} + \beta F}{k(M)}; \quad x_2 = F; \quad x_3 = M, \\ u_1 &= \frac{\ddot{F} + \beta \dot{F}}{\beta k(M)} + (\dot{F} + \beta F) \\ &\quad \times \left[\frac{1}{\beta} + \frac{1}{k(M)} - \frac{k'(M)}{\beta k^2(M)}\dot{M}\right], \\ u_2 &= \dot{M} + qM - \alpha(\dot{F} + \beta F) \end{aligned} \tag{2.3}$$

with

$$k'(M) = \frac{k_1}{M^2} k(M). \tag{2.4}$$

2.3. Multivariable Reactor System Analysis in Terms of Flatness

The *differential parametrization* (2.3) implies the following *static parametrization* for the equilibria of the system in terms of the flat output equilibria. Let $\bar{F}$ and $\bar{M}$ stand for given equilibrium values of the flat outputs, then the corresponding equilibria for the state variables and the control inputs is given by

$$\begin{aligned} \bar{x}_1 &= \frac{\beta \bar{F}}{k(\bar{M})}; \quad \bar{x}_2 = \bar{F}; \quad \bar{x}_3 = \bar{M}; \\ \bar{u}_1 &= \bar{F} + \frac{\beta \bar{F}}{k(\bar{M})}; \quad \bar{u}_2 = q\bar{M} - \alpha\beta\bar{F}. \end{aligned} \tag{2.5}$$

Thus, given a desired set of equilibrium values for the flat outputs, $\bar{y} = (\bar{F}, \bar{M}) = (\bar{x}_2, \bar{x}_3)$, the equilibrium values, $\bar{x}_1$, $\bar{u}_1$ and $\bar{u}_2$ are uniquely determined. The manifold of equilibria in the state space is readily obtained from (2.5) as the set (see Fig. 1)

$$\{x = \bar{x} \in R^3 : \bar{x}_1 k(\bar{x}_3) - \beta \bar{x}_2 = 0\}. \tag{2.6}$$

Furthermore, eliminating the constant value $\bar{F}$ in the last two expressions in (2.5) leads to the following algebraic equation:

$$q\bar{M} - \bar{u}_2 = \alpha\beta\bar{u}_1 \frac{k(\bar{M})}{k(\bar{M}) + \beta}. \tag{2.7}$$

It is easy to show that the algebraic equation (2.7) always has at least one positive stable solution for $\bar{M}$. For this, notice that $\bar{u}_1$ only magnifies, or shrinks, the distance between the possible intersection points of the positive sloped straight line, on the left-hand side of (2.7), with the "sigmoid" shaped function on the right-hand side of (2.7). However, it may be seen that for a certain positive value of $\bar{u}_2$, two equilibrium solutions may appear; a stable one, and an unstable one. As $\bar{u}_2$ is varied beyond this critical point, the unstable solution bifurcates into a high temperature stable equilibrium solution and a lower temperature unstable equilibrium solution. The last equilibrium point represents the interesting case motivating the equilibrium transfer problem to be dealt in the next section. For the range of values of $\bar{u}_1$ and $\bar{u}_2$, two stable equilibrium solutions will exist; one representing a high temperature–high conversion rate equilibrium and the second one representing a low temperature–low conversion rate equilibrium. In the middle of these two stable equilibria, there exists an intermediate temperature–intermediate conversion rate, yet unstable, equilibrium which is deemed desirable for technical and economic reasons (see Fig. 2 for details).

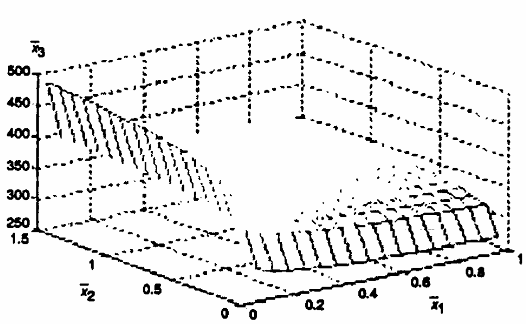

Fig. 1. Manifold of constant equilibria in the state space.

A similar analysis of the equilibria can be carried out by eliminating the constant value, $\bar{M}$, from the last two expressions in (2.5).

It also follows from the differential parametrization (2.3), that the flat outputs have a trivial *zero dynamics* (i.e., they do not have a zero dynamics). Hence, an equilibrium transfer problem, defined in terms of suitable smooth trajectories for such variables, results in a stable closed loop system devoid of such zero dynamics. It is clear from (2.1) or (2.3), that the variables x_1 and x_3 are *vector relative degree* (1, 1), with x_1 and x_3 also being minimum phase outputs (i.e., x_1 and x_3 are *passive outputs*). Indeed, letting $x_1 = \bar{x}_1$ and $x_3 = \bar{x}_3 = \bar{M}$ to be constants, we obtain the following differential equation for the corresponding zero dynamics for F, i.e., for x_2:

$$\dot{F} = -\beta\left(F - \frac{k(\bar{M})\bar{x}_1}{\beta}\right) \tag{2.8}$$

which clearly shows that F is asymptotically stable to the corresponding equilibrium point $\bar{F} = k(\bar{M})\bar{x}_1/\beta$. Therefore, the variables x_1 and x_3 are minimum phase outputs.

The differential parametrization also allows one to establish the local, or global, *detectability*, as defined in [3], of a given equilibrium state, $\bar{x}$ (see also the Appendix). Consider the passive outputs (x_1, x_3) as the system outputs, $z = h(x) = (x_1, x_3)$. According to (2.6), the equilibrium state, corresponding to constant values of the output components, is given by $\bar{x} = (\bar{x}_1, \bar{x}_2, \bar{x}_3) = (\bar{x}_1, k(\bar{x}_3)\bar{x}_1/\beta, \bar{x}_3)$. Moreover, the constant values of the inputs, corresponding to this equilibrium state are given by $(\bar{u}_1, \bar{u}_2) = ((k(\bar{x}_3) + \beta)\bar{x}_1/\beta, q\bar{x}_3 - \alpha k(\bar{x}_3)\bar{x}_1)$.

Choose an arbitrary initial state vector $x(t_0)$ located on the manifold $Z = \{x \in R^3 \mid z = \bar{z} = (\bar{x}_1, \bar{x}_3)\}$, i.e., $x(t_0)$ is of the form $x(t_0) = (\bar{x}_1, x_2(t_0), \bar{x}_3)$, with $x_2(t_0)$ being arbitrary. The motions of the system, restricted to the manifold Z (i.e. the motions of $x_2 = F$), when

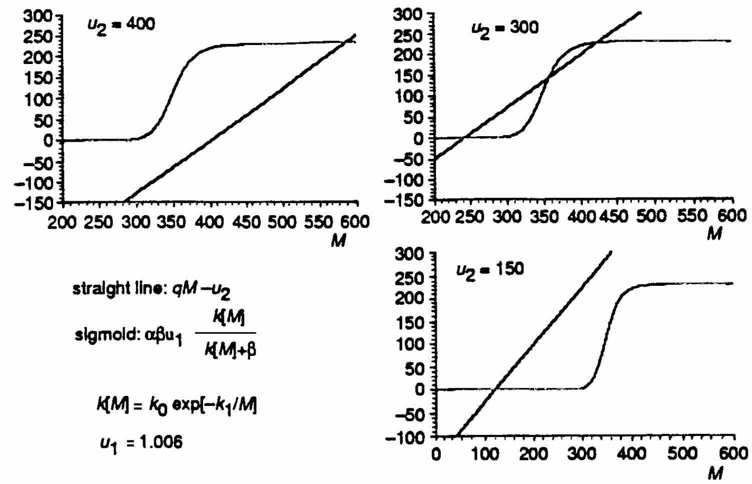

Fig. 2. Parametrization of reactor temperature equilibria in terms of constant control input values.

such motions are started on Z, with the applied control input vector given by the constant value $\bar{u} = (\bar{u}_1, \bar{u}_2)$, are governed, according to the differential parametrization (2.3), by the dynamics

$$\ddot{F} + (k(\bar{x}_3) + 2\beta)\dot{F} + \beta(\beta + k(\bar{x}_3))\left[F - \frac{k(\bar{x}_3)\bar{x}_1}{\beta}\right] = 0 \qquad (2.9)$$

which represents an asymptotically stable second order, time invariant, linear system, with constant equilibrium point given by $\bar{F} = \bar{x}_2 = \bar{x}_1 k(\bar{x}_3)/\beta$, which is the expected equilibrium value of x_2. Since this behaviour is independent of the initial condition for $F(t_0) = x_2(t_0)$, the system is globally *equilibrium state detectable* from the passive outputs.

It is also true, that the flat outputs $(F, M) = (x_2, x_3)$, taken as the system outputs $z = (x_2, x_3)$ are trivially *globally equilibrium state observable*, according to the definition given in the Appendix.

In general, many important system properties may be inferred from the differential parametrization provided by the differential flatness of a system.

3. A Passivity-Based Controller for the Reactor Model

Consider the following positive definite *storage function* $V(x)$ given by

$$V(x) = \tfrac{1}{2}(x_1^2 + x_2^2 + x_3^2). \qquad (3.1)$$

The time derivative of $V(x)$ along the controlled trajectories of the reactor system (2.1) are given by

$$\dot{V}(x) = -(k(x_3) + \beta)x_1^2 - \beta x_2^2 - qx_3^2 + x_1[\beta u_1 + k(x_3)x_2] + x_3[u_2 + \alpha k(x_3)x_1]. \qquad (3.2)$$

It is evident that the following input coordinate transformation, or static state feedback

$$v_1 = \beta u_1 + k(x_3)x_2; \quad v_2 = u_2 + \alpha k(x_3)x_1 \qquad (3.3)$$

renders the system state variables x_1, x_3, as passive outputs. Indeed, letting $z^T = [x_1 \ x_3]$ and $v = [v_1 \ v_2]^T$, we have, from (3.2) and (3.3), that, for all x, the following *infinitesimal form* of the basic passivity inequality (see [3]) is satisfied

$$\dot{V} \leq x_1 v_1 + x_3 v_2 = z^T v.$$

In new input coordinates, v_1, v_2, the system, with output vector z, may be rewritten in *Hamiltonian* form, including the dissipation structure (see [17]) as

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} 0 & -k(x_3) & 0 \\ k(x_3) & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} - \begin{bmatrix} k(x_3)+\beta & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & q \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

$$z=\begin{bmatrix}1 & 0 & 0\\ 0 & 0 & 1\end{bmatrix}\quad x=\begin{bmatrix}x_1\\ x_3\end{bmatrix}. \tag{3.4}$$

Let R_{i1}, R_{i2}, R_{i3} be strictly positive design constants representing suitable "damping injection" gains. Consider then, the following *auxiliary*, linear, time varying, controlled system

$$\begin{aligned}\begin{bmatrix}\dot{x}_{1a}\\ \dot{x}_{2a}\\ \dot{x}_{3a}\end{bmatrix} &= \begin{bmatrix}0 & -k(x_3) & 0\\ k(x_3) & 0 & 0\\ 0 & 0 & 0\end{bmatrix}\begin{bmatrix}x_{1a}\\ x_{2a}\\ x_{3a}\end{bmatrix}\\ &\quad-\begin{bmatrix}k(x_3)+\beta & 0 & 0\\ 0 & \beta & 0\\ 0 & 0 & q\end{bmatrix}\begin{bmatrix}x_{1a}\\ x_{2a}\\ x_{3a}\end{bmatrix}\\ &\quad+\begin{bmatrix}R_{i1} & 0 & 0\\ 0 & R_{i2} & 0\\ 0 & 0 & R_{i3}\end{bmatrix}\begin{bmatrix}x_1-x_{1a}\\ x_2-x_{2a}\\ x_3-x_{3a}\end{bmatrix}\\ &\quad+\begin{bmatrix}1 & 0\\ 0 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}v_1\\ v_2\end{bmatrix}\end{aligned} \tag{3.5}$$

Define a state trajectory tracking error vector e as, $e^{\mathrm{T}}=[e_1,e_2,e_3]=[(x_1-x_{1a}),(x_2-x_{2a}),(x_3-x_{3a})]$. One readily obtains from (3.4) and (3.5) that the error vector satisfies the following time-varying, *linear* system of differential equations:

$$\begin{aligned}\begin{bmatrix}\dot{e}_1\\ \dot{e}_2\\ \dot{e}_3\end{bmatrix} &= \begin{bmatrix}0 & -k(x_3) & 0\\ k(x_3) & 0 & 0\\ 0 & 0 & 0\end{bmatrix}\begin{bmatrix}e_1\\ e_2\\ e_3\end{bmatrix}\\ &\quad-\begin{bmatrix}k(x_3)+\beta+R_{i1} & 0 & 0\\ 0 & \beta+R_{i2} & 0\\ 0 & 0 & q+R_{i3}\end{bmatrix}\\ &\quad\times\begin{bmatrix}e_1\\ e_2\\ e_3\end{bmatrix}\end{aligned} \tag{3.6}$$

The modified, or shapped, storage function

$$\begin{aligned}V(e) &= \tfrac{1}{2}(e_1^2+e_2^2+e_3^2)\\ &= \tfrac{1}{2}[(x_1-x_{1a})^2+(x_2-x_{2a})^2\\ &\quad+(x_3-x_{3a})^2]\end{aligned} \tag{3.7}$$

exhibits a negative definite time derivative along the controlled solutions of systems (3.4) and (3.5). Indeed

$$\begin{aligned}\dot{V}(e) &= -k(x_3)e_1^2-[(\beta+R_{i1})e_1^2+(\beta+R_{i2})e_2^2\\ &\quad+(q+R_{i3})e_3^2]\\ &\le -[(\beta+R_{i1})e_1^2+(\beta+R_{i2})e_2^2\\ &\quad+(q+R_{i3})e_3^2]\\ &\le -\frac{\gamma}{\lambda}V(e),\end{aligned} \tag{3.8}$$

where γ and λ are strictly positive quantities given, by virtue of the positive nature of q and β by

$$\gamma=\max\{1,(\beta+R_{i1}),(\beta+R_{i2}),(q+R_{i3})\};$$
$$\lambda=\min\{1,(\beta+R_{i1}),(\beta+R_{i2}),(q+R_{i3})\}.$$

The error vector e asymptotically exponentially converges to zero and the plant state variables x_1, x_2 and x_3 asymptotically exponentially converge towards the auxiliary variables x_{1a}, x_{2a}, x_{3a}, independently of the control inputs v.

The "energy shapping plus damping injection" controller design method is based upon regarding the auxiliary system (3.5) as an *exogenous* system which is capable of "pulling" the plant trajectories towards desired equilibria. Notice that the auxiliary variables x_{1a} and x_{3a} are also relative degree (1, 1), minimum phase, variables themselves and, hence, they are also passive variables on which desired trajectories, $x_1^*(t)$, $x_3^*(t)$, can be imposed at will. The corresponding feedback controller can be computed, in this case, by straightforward system inversion, without any risks of having a closed loop unstable system. Furthermore, since the auxiliary system is created by the designer, the auxiliary system state variables can be given *any* set of convenient initial conditions in correspondence with the prescribed trajectories. The resulting *zero dynamics* of the controlled auxiliary system is represented by the closed loop evolution of the variable x_{2a}, which for convenience we denote by ξ from now on. The required control inputs v_1 and v_2 are, therefore, obtained from (3.5) as

$$\begin{aligned}v_1 &= \dot{x}_1^*(t)+k(x_3)\xi+(k(x_3)+\beta)x_1^*(t)\\ &\quad-R_{i1}(x_1-x_1^*(t)),\\ v_2 &= \dot{x}_3^*(t)+qx_3^*(t)-R_{i3}(x_3-x_3^*(t)).\end{aligned} \tag{3.9}$$

When the feedback loop is closed around the auxiliary system with the control law (3.9), it is also closed on the nonlinear plant, given that the auxiliary system shares the control inputs with the plant. Since the initial conditions, $x_{1a}(t_0)$, $x_{2a}(t_0)$, $x_{3a}(t_0)$ of the auxiliary system are chosen at will, those corresponding with the passive outputs may be prescribed as $x_{1a}(t_0) = x_1^*(t_0)$ and $x_{3a}(t_0) = x_3^*(t_0)$. Hence, the auxiliary variables $x_{1a}(t)$ and $x_{3a}(t)$ identically follow the open loop prescribed signals $x_1^*(t), x_3^*(t)$, irrespectively of the evolution of the plant state $x(t)$ and the auxiliary system remaining variable $\xi(t)$. The initial condition for x_{2a} i.e., $x_{2a}(t_0) = \xi(t_0)$ may be arbitrarily chosen and its evolution, representing a minimum phase outputs stable zero dynamics, is determined by

$$\dot{\xi} = k(x_3)x_1^*(t) - \beta\xi + R_{t2}(x_2 - \xi). \tag{3.10}$$

Equation (3.10), in combination with (3.9), effectively represent a dynamical feedback controller for the original plant.

The controlled motions of x_2 were seen to converge towards those of ξ and these, in turn, are seen to converge, according to (3.10), towards, $\bar{\xi} = k(\bar{x}_3^*)\bar{x}_1^*/\beta$, with $\bar{x}_1^*$ and $\bar{x}_3^*$ being the desired final equilibrium values prescribed by the planned trajectories $x_1^*(t)$ and $x_3^*(t)$. This, however, is the same equilibrium point for x_2, as it can be deduced from (2.5).

Notice that, in the ideal case, when the initial states of the plant precisely coincide with the initial states of the auxiliary system and these, in turn, are set, precisely, at the initial values of the passive outputs prescribed trajectories and, of course, there are no external perturbations and no plant parameter variations, then the controller state ξ exactly coincides with the ideal trajectory of the plant state $x_2 = x_2^*(t)$ and, naturally, the passive outputs x_1 and x_3 exactly coincide with the prescribed trajectories, $x_1^*(t)$ and $x_3^*(t)$. Under these conditions, the *nominal* passivity based controller satisfies the following expressions:

$$\begin{aligned} v_1^*(t) &= \dot{x}_1^*(t) + k(x_3^*(t))x_2^*(t) \\ &\quad + (k(x_3^*(t)) + \beta)x_1^*(t), \\ v_2^*(t) &= \dot{x}_3^*(t) + qx_3^*(t) \end{aligned} \tag{3.11}$$

with

$$\begin{aligned} u_1^*(t) &= \frac{1}{\beta}(v_1^*(t) - k(x_3^*(t))x_2^*(t)); \\ u_2^*(t) &= v_2^*(t) - \alpha k(x_3^*(t))x_1^*(t). \end{aligned} \tag{3.12}$$

3.1. An Equilibrium Transfer Via Trajectory Planning for the Passive Outputs

The control objective consist in regulating the states from a given constant stable equilibrium point at time t_1, $x(t_1) = \bar{x}_{in} = (\bar{x}_{1in}, \bar{x}_{2in}, \bar{x}_{3in})$, towards a second, unstable, equilibrium point $x(t_2) = \bar{x}_f = (\bar{x}_{1f}, \bar{x}_{2f}, \bar{x}_{3f})$, in a prespecified amount of time $\Delta = t_2 - t_1 > 0$. This objective may be achieved by means of a corresponding transfer of the minimum phase outputs, x_1 and x_3, from the initial equilibrium values, $\bar{x}_{1in}$ and $\bar{x}_{3in}$, towards the final equilibrium values, $\bar{x}_{1f}$ and $\bar{x}_{3f}$. Due to the minimum phase character of the passive outputs, the regulation of the passive outputs indirectly and stably regulates the remaining variable x_2 from the initial equilibrium value x_{2in} towards the desired equilibrium value x_{2f}.

A set of open loop trajectories $x_1^*(t)$ and $x_3^*(t)$ for the passive auxiliary outputs x_{1a} and x_{3a}, achieving a transfer between the two equilibrium points $(\bar{x}_{1in}, \bar{x}_{3in})$ and $(\bar{x}_{1f}, \bar{x}_{3f})$, may be specified in terms of suitable polynomials, as follows:

$$\begin{aligned} x_1^*(t) &= \bar{x}_{1in} + \left[252\left(\frac{t-t_1}{\Delta}\right)^5 - 1050\left(\frac{t-t_1}{\Delta}\right)^6 \right. \\ &\quad + 1800\left(\frac{t-t_1}{\Delta}\right)^7 - 1575\left(\frac{t-t_1}{\Delta}\right)^8 \\ &\quad \left. + 700\left(\frac{t-t_1}{\Delta}\right)^9 - 126\left(\frac{t-t_1}{\Delta}\right)^{10}\right] \\ &\quad \times (\bar{x}_{1f} - \bar{x}_{1in}), \\ x_3^*(t) &= \bar{x}_{3in} + \left[252\left(\frac{t-t_1}{\Delta}\right)^5 - 1050\left(\frac{t-t_1}{\Delta}\right)^6 \right. \\ &\quad + 1800\left(\frac{t-t_1}{\Delta}\right)^7 - 1575\left(\frac{t-t_1}{\Delta}\right)^8 \\ &\quad \left. + 700\left(\frac{t-t_1}{\Delta}\right)^9 - 126\left(\frac{t-t_1}{\Delta}\right)^{10}\right] \\ &\quad \times (\bar{x}_{3f} - \bar{x}_{3in}). \end{aligned} \tag{3.13}$$

This particular choice of trajectories for the passive auxiliary outputs x_{1a} and x_{3a}, guarantees that at time t_1, the first four time derivatives of $x_1^*(t)$ and $x_3^*(t)$ are all zero, while at time t_2 the first five time derivatives of the planned passive outputs are also zero, thus avoiding noticeable discontinuities in the dynamically generated control inputs u_1 and u_2.

Notice that in the plane of coordinates (x_{1a}, x_{3a}), the above trajectory corresponds to a straight line starting at the point $(\bar{x}_{1in}, \bar{x}_{3in})$ and ending at the point $(\bar{x}_{1f}, \bar{x}_{3f})$. Eliminating the time parameter t in (3.13) one obtains

$$x_{3a} = \bar{x}_{3in} + \left[\frac{\bar{x}_{3f} - \bar{x}_{1in}}{\bar{x}_{1f} - \bar{x}_{1in}}\right](x_{1a} - \bar{x}_{1in}).$$

One proceeds to use the dynamical controller (3.9) and (3.10), with the planned trajectories (3.13), along with the inverse of the input coordinate transformation (3.3).

3.2. Simulation Results

Using the multivariable state feedback control scheme (3.3), (3.9) and (3.10), the previously described operating equilibrium transfer was attempted. The initial stable equilibrium point was taken, after [18] as

$$\bar{x}_{in} = (0.002, 1.1, 467.8)$$

while the unstable target equilibrium point was taken to be

$$\bar{x}_f = (0.7159, 0.29, 337.1).$$

The transfer was set to smoothly begin at $t_1 = 6$ min, and it was prescribed to be completed at $t_2 = 16$ min. The simulation results, shown in Fig. 3, correspond to the following set of system parameter values, taken from [18]

$$k_0 = 7.2 \times 10^{10}; \quad k_1 = 8700; \quad \beta = 1.1;$$
$$\alpha = 209.2; \quad q = 1.25.$$

The controller design parameters were chosen as

$$R_{i1} = 2; \quad R_{i2} = 2; \quad R_{i3} = 2.$$

The simulations show that the unrestricted passivity based controller (3.9), (3.10) and (3.13) manages to achieve the desired equilibrium transfer for all three plant state variables (x_1, x_2, x_3), but at the expense of a substantial increase of the feed concentration input during the transfer maneuver and, also, of an unrealistic feed plus coolant temperature profile. This behaviour is independent of the design values R_{i1}, R_{i2}, R_{i3} and of the time interval $\Delta = t_2 - t_1$. The induced trajectory on the product concentration state variable x_2 presents an unacceptably high increase during the transient phase of the planned equilibrium transfer. Moreover, when the physically meaningful magnitude restrictions on the inputs (see [18])

$$u_1 \in [u_{1\,\min}, u_{1\,\max}] = \left[0, x_1^{\text{feed}}\right] = [0, 1.102];$$
$$u_2 \in [u_{2\,\min}, u_{2\,\max}] = [300, 500]$$

are enforced, the passivity based controller leads the state trajectories towards an undesired equilibrium point.

The proposed passivity based controller, with the prescribed reference trajectories for the passive outputs, fails to directly achieve the required equilibrium transfer within physically meaningful values

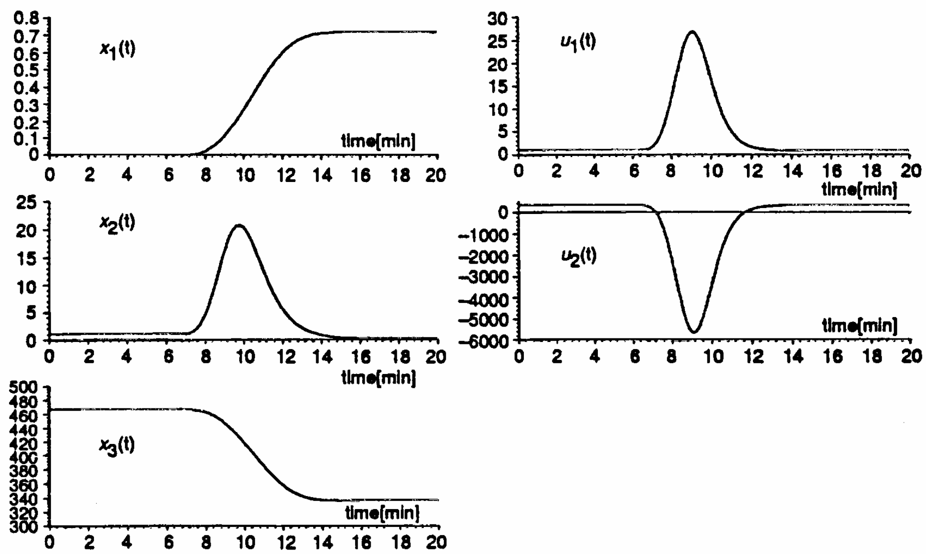

Fig. 3. Simulation results for exothermic reactor unfeasible equilibrium transfer by means of a passivity based controller with planning of passive outputs trajectories.

for the control inputs and the product concentration, specially if the control input magnitudes are unrestricted.

4. An Exact Linearization Based Controller for the Multivariable Reactor Model

4.1. An Equilibrium Transfer Via Trajectory Planning for the Flat Outputs

The equilibrium transfer objective described in the previous section will now be attempted by means of a corresponding transfer of the flat outputs, instead of the passive outputs. The initial equilibrium values, $F(t_1) = \bar{F}_{\text{in}} = \bar{x}_{2\text{in}}$ and $M(t_1) = \bar{M}_{\text{in}} = \bar{x}_{3\text{in}}$, will be transfered towards the final equilibrium values, $F(t_2) = \bar{F}_f = \bar{x}_{2f}$ and $M(t_2) = \bar{M}_f = \bar{x}_{3f}$. Thanks to the absence of zero dynamics for the flat outputs, and the static relationship (2.5), the regulation of the flat outputs indirectly, and stably, regulates the remaining variable x_1, from the initial equilibrium value, $x_{1\text{in}}$, towards the desired final equilibrium value, x_{1f}. Both values are uniquely determined from the corresponding equilibrium values $\bar{F}, \bar{M}$, of the flat outputs, as in (2.5).

A set of open loop trajectories $F^*(t)$ and $M^*(t)$ for the flat outputs F and M, achieving a transfer between the two equilibrium points $(\bar{F}_{\text{in}}, \bar{M}_{\text{in}})$ and $(\bar{F}_f, \bar{M}_f)$, may be specified in terms of suitable polynomials as before. The next step is to impose on the flat output tracking errors, $e_F(t) = F - F^*(t)$ and $e_M(t) = M - M^*(t)$, the following linear, time-invariant, asymptotically stable behaviours:

$$\begin{aligned} \ddot{e}_F(t) + a_1\dot{e}_F(t) + a_0 e_F(t) &= 0, \\ \dot{e}_M(t) + b_0 e_M(t) &= 0, \end{aligned} \tag{4.1}$$

where the sets of coefficients $\{a_1, a_0\}$ and $\{b_0\}$ are chosen so that the corresponding polynomials in the complex variable s,

$$p_F(s) = s^2 + a_1 s + a_0; \quad p_M(s) = s + b_0 \tag{4.2}$$

are both *Hurwitz* polynomials, i.e., with all their roots having strictly negative real parts.

The specification of the tracking errors dynamics (4.1) and the use of the expressions for u_1 and u_2 in (2.3), results in the following feedback controller explicitly based on the off-line specification of the flat outputs reference trajectories:

$$\begin{aligned} u_1 &= \frac{\ddot{F}^*(t) - a_1(\dot{F} - \dot{F}^*(t)) - a_0(F - F^*(t)) + \beta\dot{F}}{\beta k(M)} \\ &\quad + (\dot{F} + \beta F)\left[\frac{1}{\beta} + \frac{1}{k(M)} - \frac{k'(M)}{\beta k^2(M)}\dot{M}\right] \\ u_2 &= \dot{M}^*(t) - b_0(M - M^*(t)) + qM \\ &\quad - \alpha(\dot{F} + \beta F). \end{aligned} \tag{4.3}$$

4.2. Simulation Results

Using the multivariable state feedback control scheme (4.3), the above described operating equilibrium transfer was attempted between the same operating equilibrium points as in the previous section, and using the same system parameter values for the reactor system.

For simplicity, we prescribed for the flat outputs similar time polynomials, as those used in the previous section. These were set to be

$$\begin{aligned} F^*(t) &= \bar{F}_{\text{in}} + \left[252\left(\frac{t-t_1}{\Delta}\right)^5 - 1050\left(\frac{t-t_1}{\Delta}\right)^6 \right. \\ &\quad + 1800\left(\frac{t-t_1}{\Delta}\right)^7 - 1575\left(\frac{t-t_1}{\Delta}\right)^8 \\ &\quad \left. + 700\left(\frac{t-t_1}{\Delta}\right)^9 - 126\left(\frac{t-t_1}{\Delta}\right)^{10}\right] \\ &\quad \times (\bar{F}_f - \bar{F}_{\text{in}}), \\ M^*(t) &= \bar{M}_{\text{in}} + \left[252\left(\frac{t-t_1}{\Delta}\right)^5 - 1050\left(\frac{t-t_1}{\Delta}\right)^6 \right. \\ &\quad + 1800\left(\frac{t-t_1}{\Delta}\right)^7 - 1575\left(\frac{t-t_1}{\Delta}\right)^8 \\ &\quad \left. + 700\left(\frac{t-t_1}{\Delta}\right)^9 - 126\left(\frac{t-t_1}{\Delta}\right)^{10}\right] \\ &\quad \times (\bar{M}_f - \bar{M}_{\text{in}}). \end{aligned} \tag{4.4}$$

The controller design parameters were chosen so that the polynomial $p_F(s)$ had, both, roots located at the point, $-2 + 0j$, of the real axis in the complex plane, while the only root of the polynomial $p_M(s)$ was set to lie at the same point $-2 + 0j$ of the complex plane i.e.

$$a_1 = 4; \quad a_0 = 4; \quad b_0 = 2.$$

The simulation results shown in Fig. 4, clearly show that the linearizing controller based on flatness

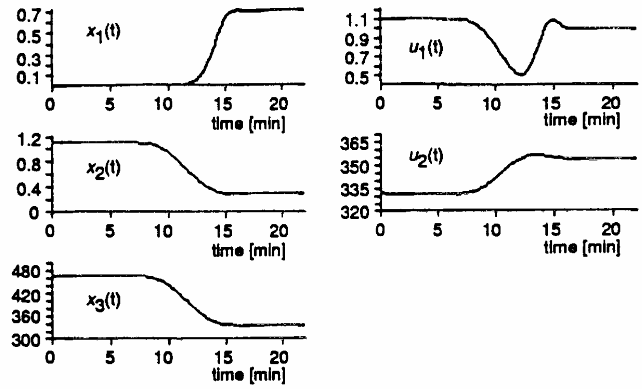

Fig. 4. Simulation results for exothermic reactor feasible equilibrium transfer by means of planned flat outputs trajectory tracking errors linearization.

manages to suitably transfer the high-temperature equilibrium point towards the intermediate temperature unstable equilibrium point. This maneuver is achieved thanks to the fact that the control actions result in a suitable "cooling off" of the reactor. This is achieved without shutting off the reactant concentration at the feed and, also, without saturation of any of the two control inputs, nor obtaining unrealistic state behaviour or unfeasible control manoeuvers.

5. A Passivity Based Controller with Planned Flat Outputs Trajectories

In order to combine the physically oriented nature of the passivity based controller with the demonstrated effectiveness of the LF controller, the passivity based controller (3.3), (3.9) and (3.10) was still implemented but now making use of the relation existing between the flat outputs F and M and the passive outputs x_1 and x_3, as given by (2.3)

$$x_1 = \frac{\dot{F} + \beta F}{k(M)}; \quad x_3 = M. \tag{5.1}$$

Thus, instead of directly using the planned trajectories, $x_1^*(t)$ and $x_3^*(t)$, in the passivity based controller (3.9) and (3.10), these were substituted by

$$x_1^*(t) = \frac{\dot{F}^*(t) + \beta F^*(t)}{k(M^*(t))}; \quad x_3^*(t) = M^*(t) \tag{5.2}$$

with the planned flat outputs, $F^*(t)$ and $M^*(t)$, given as in (4.4).

The proposed PF controller basically forces the state variables x_1 and x_3 to follow the natural *image trajectories* that correspond with the planned flat outputs trajectories, $F^*(t)$ and $M^*(t)$, via the differential parameterization allowed by the flatness property of the system. Therefore, in essence, a similar type of behaviour, as obtained in the linearizing tracking error controller of the previous section, is expected for the product concentration variable x_2, thus avoiding its inconvenient increase during the operating point transfer. The fundamental difference of the PF controller with the LF controller, lies in the fact that the trajectory tracking errors, while still being linear and asymptotically exponentially stable to zero (see (3.6)), they no longer obey independent (decoupled) dynamics nor are they time-invariant as in (4.1). In fact, one of the possible advantages accounting for the simplicity of the passivity based controller is that no extra effort is needed to decouple the tracking errors or to make them evolve in a time-invariant fashion. The PF tends to exploit the system structure by, first, respecting the natural – usually beneficial – damping and workless structure of the system, while eliminating, via partial feedback, only those nonlinear forces which are locally destabilizing. Secondly, the enhancement of the original damping structure of the system, through linear, dissipative, tracking error injection, is carried out only if deemed necessary.

5.1. Ideal Equivalence of the PF and the LF Trajectory Tracking Controllers

The simulations depicting the performance of the PF based controller accomplish the proposed operating equilibrium transfer, described in the previous section, exactly in the same manner as the LF based controller provided no initial setting errors are allowed and, of course, the same planned trajectories are used for the flat outputs in both cases. The explanation of this coincidence in the ideal behaviours is quite simple if one considers the linearizing controller expressions (4.3) under the assumption of zero initial tracking error and no parametric perturbations. Letting $M(t) = M^*(t) = x_3^*(t)$, $F(t) = F^*(t) = x_2^*(t)$ and using the relations (2.3) and (2.4), one obtains from (4.3), the following string of equalities:

$$\begin{aligned}
u_1^*(t) &= \frac{\ddot{F}^*(t) + \beta\dot{F}^*(t)}{\beta k(M^*(t))} + (\dot{F}^*(t) + \beta F^*(t)) \\
&\quad \times \left[\frac{1}{\beta} + \frac{1}{k(M^*(t))} - \frac{k'(M^*(t))}{\beta k^2(M^*(t))}\dot{M}^*(t)\right] \\
&= \frac{\ddot{x}_2^*(t) + \beta\dot{x}_2^*(t)}{\beta k(x_3^*(t))} + (\dot{x}_2^*(t) + \beta x_2^*(t)) \\
&\quad \times \left[\frac{1}{\beta} + \frac{1}{k(x_3^*(t))} - \frac{k'(x_3^*(t))}{\beta k^2(x_3^*(t))}\dot{x}_3^*(t)\right] \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\dot{x}_2^*(t) + \beta x_2^*(t)}{\beta k(x_3^*(t))}\right) \\
&\quad + \frac{1}{\beta}(k(x_3^*(t)) + \beta)x_1^*(t) \\
&= \frac{1}{\beta}(\dot{x}_1^*(t) + (k(x_3) + \beta)x_1^*(t) \\
&\quad + k(x_3^*(t))x_2^*(t) - k(x_3^*(t))x_2^*(t)) \\
&= \frac{1}{\beta}(v_1^*(t) - k(x_3^*(t))x_2^*(t)). \\
u_2^*(t) &= \dot{M}^*(t) + qM^*(t) - \alpha(\dot{F}^*(t) + \beta F^*(t)) \\
&= \dot{x}_3^*(t) + qx_3^*(t) - \alpha k(x_3^*(t))x_1^*(t) \\
&= v_2^*(t) - \alpha k(x_3^*(t))x_1^*(t)
\end{aligned} \tag{5.3}$$

which are just the corresponding expressions for the passivity based controller (3.3) and (3.9), under ideal (nominal) tracking conditions, given in (3.11) and (3.12). For this reason, we do not reproduce the corresponding simulations here and refer to those already presented in Fig. 4 for the LF controller ideal performance. However, the tracking error behaviours of both controllers is quite different when initial conditions are not ideally set at the operating equilibrium and the plant parameters vary in an unforseeable fashion during the equilibrium transfer operation.

5.2. Performance Comparison, Under Initial State Setting Erros and Parameter Variations, of the LF and the PF Controllers

In order to compare the performance of both controllers when initial state perturbations are present, we show in Figs. 5 and 6 the stabilizing features of both controllers for the same perturbations of the initial conditions around the initial stable equilibrium point. We adopted, as a testing condition, a 10% discrepancy of all the initial states with respect to the ideal initial operating equilibrium point.

While the PF controller manages to stabilize the controlled trajectories to the ideal initial conditions, the response may unrealistically adopt negative transient values for the reactant concentration if no control input limitations are enforced. This feature is also shared by the exact linearization tracking controller, but for substantially higher perturbations of the initial conditions. When saturation limits are enforced over the control input signals, the simulations shown in Fig. 5 show that the PF controller initially exhibits a "bang bang" behaviour in both control input signals u_1, u_2. This is not the case of the LF controller which, also after a very fast state transient (not noticeable in the presented simulations), devoid of controller saturations, proceeds to smoothly reach the nominal operating value of the control inputs, corresponding to the initial equilibrium point.

The reasons behind this transient behaviour lies in the fact that the time varying energy dissipation term in the reactant concentration subsystem (i.e., the term of the form: $-k(x_3)x_1$) tends to be exceedingly large at the initial operating point. The passivity based controller, with planned flat outputs, does not compensate this large quantity and rather tends to let the system "overreact" to initial setting errors thus causing the control inputs to rapidly reach their saturation limits. This feature is not present in the LF based controller. Its closed loop performance is devoid of control saturations. In this respect, the PF controller, although equally as effective as the LF controller in achieving the desired transfer is not as well behaved regarding transient behaviour and respecting saturations limits. Larger initial state deviations tend to rapidly destabilize the closed loop behaviour of the PF controlled system, while that of the linearization based controller is still well behaved and effective.

The effect of unmodelled, time-dependent, variations in all of the three constant parameters entering the description of the reactor model (2.1) was also investigated. In order to compare the closed loop performances of the two controllers, we propose the following "benign" (i.e. smooth and temporary)

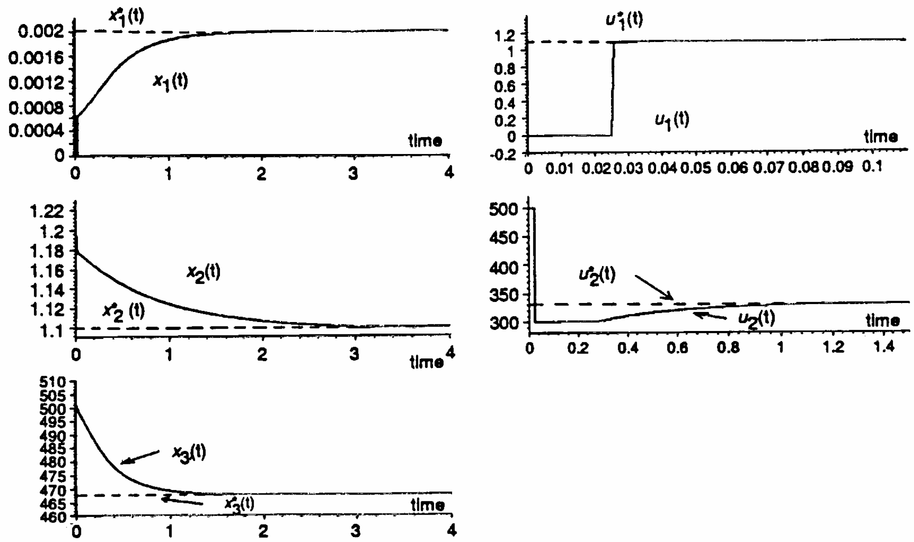

Fig. 5. Closed loop trajectory tracking errors for initial state setting errors: Passivity plus flatness based controller.

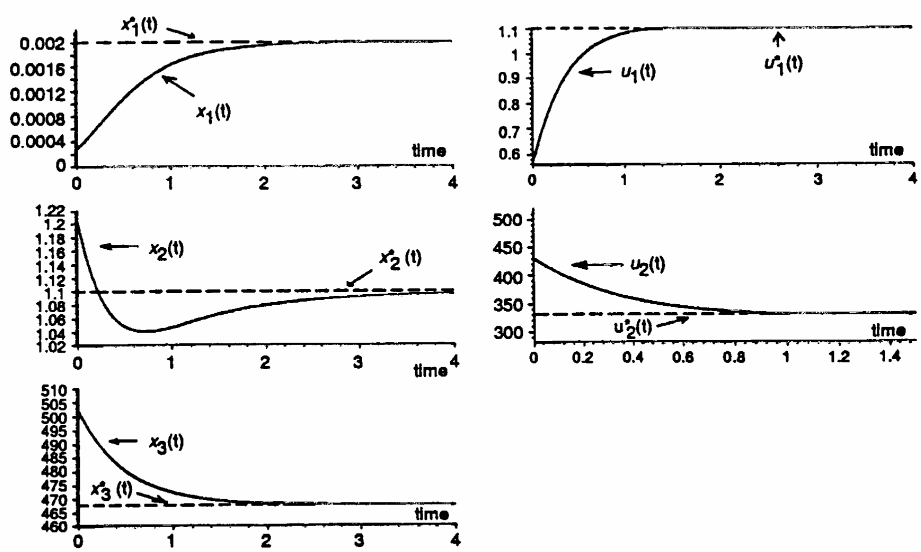

Fig. 6. Closed loop trajectory tracking errors for initial state setting errors: Linearization plus flatness based controller.

variations of the reactor constants, α, β and q, in the form of gaussian shaped functions, centered, all of them, around the midpoint t_m of the equilibrium transfer interval, $[t_1, t_2]$, i.e. $t_m = 0.5(t_1 + t_2)$, with perturbation durations covering totally, or partially, the maneuvering interval, $[t_1, t_2]$. We prescribed the following time functions:

$$\tilde{\alpha}(t) = \alpha\left(1 - k_\alpha \exp\left(-\frac{(t - t_m)^2}{\sigma_\alpha^2}\right)\right)$$

$$\text{for } t \in [t_{1\alpha}, t_{2\alpha}] \subset [t_1, t_2],$$

$$\tilde{\beta}(t) = \beta\left(1 + k_\beta \exp\left(-\frac{(t-t_m)^2}{\sigma_\beta^2}\right)\right)$$
$$\text{for } t \in [t_{1\beta}, t_{2\beta}] \subset [t_1, t_2],$$
$$\tilde{q}(t) = q\left(1 - k_q \exp\left(-\frac{(t-t_m)^2}{\sigma_q^2}\right)\right)$$
$$\text{for } t \in [t_{1q}, t_{2q}] \subset [t_1, t_2],$$

where the constants k_α, k_β and k_q represent the maximum, instantaneous, allowed percent variation of the different parameters from their nominal values (these percentage constants are preceeded by a positive sign, if the variation is incremental, or by a negative sign, if it is decremental). The constants, σ_α, σ_β and σ_q, represent the "spread" of the parameter deviation around its maximum central value. The proposed parameter variations were only ascribed to the plant model but not to the controllers expressions. These parameter variations, however benign, do cause large state deviations from the prescribed nominal state trajectories.

The perturbed system responses to the LF controller actions are shown in Fig. 7. For these simulations we set: $t_m = 11$, $[t_1, t_2] = [6, 16]$ and $k_\alpha = 0.4$ (i.e., a maximum of 40% variation of the exothermicity constant α), with $\sigma_\alpha = \sqrt{0.2}$; $k_\beta = 0.4$ (i.e., a maximum of 40% variation of the dilution rate constant β), with $\sigma_\beta = \sqrt{0.4}$ and, finally, $k_q = 0.4$ with $\sigma_q = \sqrt{0.2}$. The time intervals of validity of these perturbations were set to be $[t_{1\alpha}, t_{2\alpha}] = [8, 14]$, $[t_{1\beta}, t_{2\beta}] = [6, 16]$ and $[t_{1q}, t_{2q}] = [6, 16]$. In spite of the large state deviations caused by the parameter perturbations, and the fact that one of the control input u_2 saturates for a significant amount of time, during the transfer maneuver, the closed loop response manages to recover the desired control objective without deviating towards undesirable equilibria.

The PF controller is not capable of sustaining the same extent of plant parameter deviations proposed for the LF controller. In fact, the computer simulations corresponding to the above specified perturbations brake down during the perturbed transfer, due to an exceedingly large instability of the closed loop response. A closed loop response, which still achieves the desired equilibrium transfer, is shown in Fig. 8. The parameters defining the plant parameter perturbations were set to be, in this case, as $t_m = 11$, $[t_1, t_2] = [6, 16]$ and $k_\alpha = 0.06$ (i.e., a maximum instantaneous deviation of only 6% of the exothermicity constant α), with $\sigma_\alpha = \sqrt{0.2}$; $k_\beta = 0.06$ (i.e., a maximum of 6% variation of the dilution rate constant β), with $\sigma_\beta = \sqrt{0.4}$ and, finally, $k_q = 0.05$ with $\sigma_q = \sqrt{0.2}$. The time intervals of validity of these perturbations were set to be the same as in the previous case. Notice that in spite of the small values of the parameter deviations, the control inputs behaviours nearly match those corresponding to the linearizing controller (which sustains a perturbation nearly seven times larger!).

The LF controller exhibits superior recovery features and robustness, with respect to the proposed parameter perturbations, than the PF based controller.

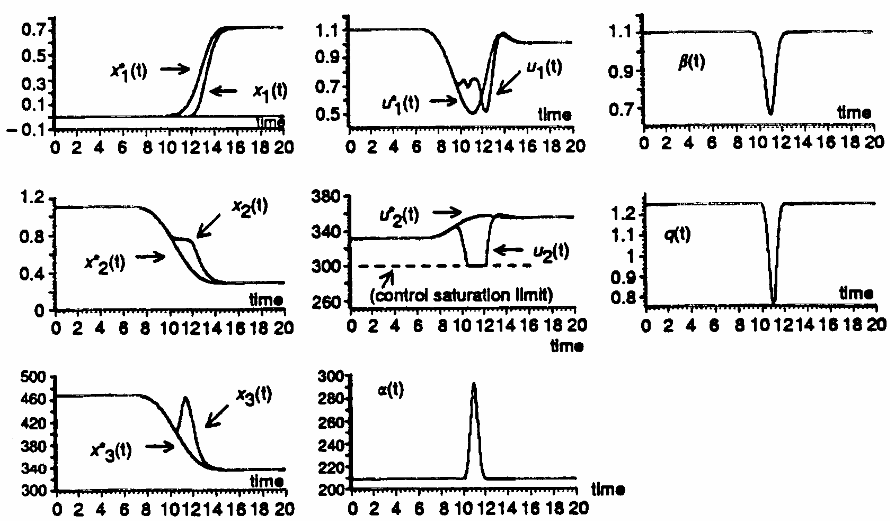

Fig. 7. Closed loop performance of linearization plus flatness controller with reactor model subject to unmodelled parameter variations (40% maximum instantaneous variation in all parameters).

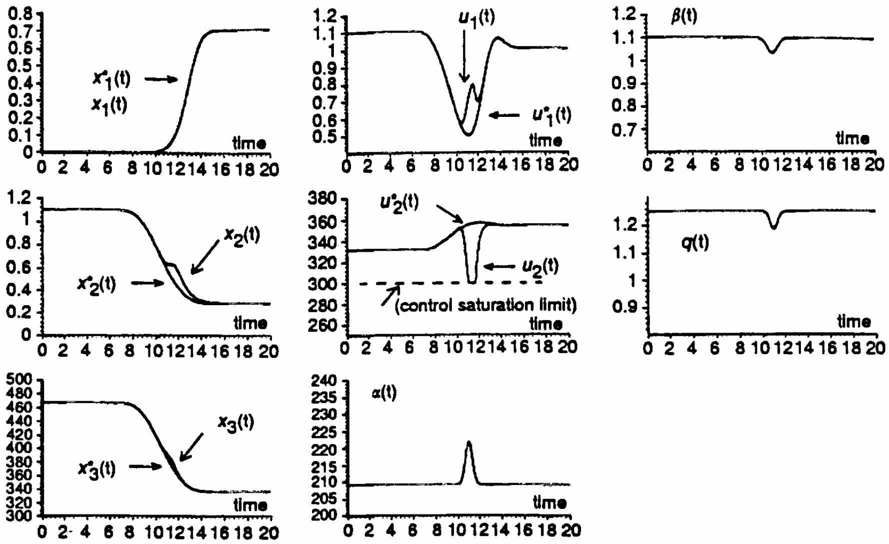

Fig. 8. Closed loop performance of passivity plus flatness controller with reactor model subject to unmodelled parameter variations (up to 6% maximum instantaneous variation in all parameters).

6. Conclusions

In this article two "stabilization by tracking" control schemes have been presented which achieve a desirable, but otherwise troublesome, equilibrium transfer in an exothermic chemical reactor subject to control input saturations. The differential flatness of the nonlinear multivariable reactor model is suitably exploited for establishing the main properties of the nonlinear plant and, also, to obtain a suitable static equilibrium parameterization which is helpful in the trajectory planning aspects of the proposed regulation approaches. Within this viewpoint of stabilization by tracking, three feedback controllers were tested. A passivity based controller with directly planned trajectories for the passive outputs, an exact feedback linearization tracking error controller, based on off-line trajectory planning for the flat outputs, and, finally, a passivity based controller using passive outputs reference trajectories which are images, under the differential parametrization map implied by flatness, of the suitable planned trajectories previously prescribed for the flat outputs. The directly designed passivity based controller was shown to fail in the realistic regulation of the system, while, both, the proposed linearizing controller and passivity based controller performed quite well. However, superior behaviour, regarding robustness to initial state setting errors and plant parameter perturbations, was exhibited by the exact linearization controller, based on flatness, over the passivity controller, based also on flatness.

The treated example has been recently examined from the perspective of "discontinuous plus hybrid" control schemes, with very interesting global asymptotic stabilization results. While the globality of our results is not discussed, controller saturations may be present for equilibrium transfers between distant operating equilibrium points. In this context, however, the stabilization by tracking approach can still be rendered valid by exploiting the off-line trajectory planning alternative combined with flatness. Flatness represents a valuable asset in such off-line planning tasks, thanks to the complete information provided by the underlying differential parametrization map. This readily allows to check for saturation conditions of nominal control inputs and the possible compliance with restrictions of the corresponding nominal state trajectories. In this same respect, a recently developed technique, known as "control of the clock", imposed on the tracking error dynamics may also be of great help in off-line trajectory planning tasks based on flatness (see Fliess et al. [6], and also Bitauld et al. [2] for interesting theoretical details and illustrative examples).

The approaches here presented may be extended to the class of multi-input, or multi-reactant, chemical reactor systems treated in [18], since it can be shown that these models are also differentially flat and passive.

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Appendix

The definitions presented in this appendix are taken from some published articles and books. Those referred to differential flatness are taken, most notably, from the articles by Prof. M. Fliess and his coworkers [4, 5], where the reader is referred for further details. The concept of passivity and feedback passivation is found in Byrnes et al. [3] and also in Ortega et al. [11] (see also [17]).

The term "variables" is taken to mean arbitrary functions of time. Differential equations are understood to be defined with respect to time differentiation.

Definition A.1. A finite set of variables, collected in a vector ξ, are said to be *differential functions* of a second set of variables, represented by the vector y, if each component of ξ is expressed in terms of the components of y and of a *finite* number of their time derivatives. We express this fact, with some abuse of notation, by writing

$$\xi = \Xi(y, \dot{y}, \dots, y^{(\alpha)}) \tag{A.1}$$

with α being a certain integer. □

Definition A.2. Let y be a set of m variables. We say that the components of y constitute a set of *differentially independent* variables if there is no differential equation relating the components of y. □

Consider a nonlinear system of the form $\dot{x} = f(x, u)$, $x \in R^n$, $u \in R^m$. Suppose a set of variables y are known to be *differential functions of the state*, i.e., $y = \eta(x, \dot{x}, \dots, x^{(\beta+1)})$ for some integer β. Then, in accordance with the prescribed system dynamics, such a differential function may be, generally speaking, written as

$$y = \eta(x, \dot{x}, \ldots, x^{(\beta+1)}) = \psi(x, u, \dot{u}, \ldots, u^{(\beta)}). \tag{A.2}$$

Definition A.3. A nonlinear system, with output vector z, given by

$$\dot{x} = f(x, u); \quad z = h(x), \quad x \in R^n, \quad z \in R^p, \quad u \in R^m \tag{A.3}$$

is said to be *differentially flat* if there exists a set of m differentially independent functions of the state, called the *flat outputs*, denoted by the vector y (i.e., $y = \psi(x, u, \dot{u}, \ldots, u^{(\beta)})$), such that all system variables (i.e., states x, outputs z, and inputs u) are, in turn, expressible as differential functions of y. In other words

$$x = A(y, \dot{y}, \ldots, y^{(\alpha)}); \quad u = B(y, \dot{y}, \ldots, y^{(\alpha+1)}); \quad z = C(y, \dot{y}, \ldots, y^{(\alpha)}). \tag{A.4}$$

□

Such a collection of differential maps is called a *differential parameterization* of the system variables, x, z, u, in terms of the components of y. Note that the number of flat outputs, m, coincides with the number of control inputs.

It should be remarked that, except for a certain collection of cases, no general criterion is known to exist which systematically may characterize a given system as a flat system. Flat outputs, however, usually enjoy a physically clear meaning (see [5] for details). Flatness represents an extension of the notion of *linear* controllability into the realm of nonlinear systems.

A given differential parametrization, such as (A.4) also allows for a *static parametrization* of the systems equilibria of the form

$$\bar{x} = A(\bar{y}, 0, \ldots, 0) = \bar{A}(\bar{y}); \quad \bar{u} = B(\bar{y}, 0, \ldots, 0) = \bar{B}(\bar{y}); \quad \bar{z} = C(\bar{y}, 0, \ldots, 0) = \bar{C}(\bar{y}). \tag{A.5}$$

Definition A.4. Let a component z_i of the output vector z of a differentially flat system be differentially parametrized by $z_i = C_i(y, \dot{y}, \ldots, y^{(\alpha)})$ with equilibrium value $\bar{z}_i = \bar{C}_i(\bar{y})$. The output z_i is said to be a (weak) *minimum phase* output around a given equilibrium value $\bar{z}_i$ if, at least locally, the implicit differential equation

$$\bar{z}_i = C_i(y, \dot{y}, \ldots, y^{(\alpha)}) \tag{A.6}$$

is (stable) asymptotically stable, around the constant solution $y = \bar{y}$.

If an output is not locally minimum phase or weakly minimum phase, then it is called a *nonminimum phase* output. The dynamics $C_i(y, \dot{y}, \ldots, y^{(\alpha)}) = \bar{z}_i$ is usually addressed as the *zero dynamics* associated with the output z_i. □

It should be clear that the flat outputs do not exhibit a zero dynamics, this is addressed by saying that the flat outputs have a *trivial* zero dynamics. This fact is exploited in the indirect regulation, and trajectory tracking tasks, for non-minimum phase outputs (see [8]).

Let $V(x)$ be a smooth positive definite scalar function, which satisfies $V(0) = 0$. Consider the nonlinear system with output vector z

$$\dot{x} = f(x, u); \quad z = h(x), \quad x \in R^n, \quad u \in R^m, \quad z \in R^m \tag{A.7}$$

i.e., the system is a *square* system.

Definition A.5 The square system (A.7) is said to be *passive* from the inputs u towards the outputs z, if, irrespectively of the initial state value $x(t_0)$, the net increase of $V(x)$, for any input vector $u(t)$ defined on $[t_0, T]$, is shown to satisfy, on any finite time interval $[t_0, T]$, the inequality constraint

$$V(x(T)) - V(x(t_0)) \leq \int_{t_0}^{T} z^T(t) u(t) \, dt.$$

□

Equivalently, the system is said to be passive if the following "inifinitesimal version" of passivity is satisfied along controlled trajectories of the system (A.7)

$$\dot{V}(x) \leq z^T u \quad \forall u.$$

In such a case, the output vector z is said to be constituted by a set of *passive outputs*. Roughly speaking, it has been shown in [3], for the case of nonlinear systems which are linear in the control inputs, that a necessary and sufficient condition for a set of outputs variables, z, to qualify as passive outputs, they must be *vector relative degree* equal to $\{1, 1, \ldots, 1\}$ and weakly *minimum phase*. In other words, the first order time derivative of the vector z is related to the set of inputs, u, via a square and invertible matrix and the corresponding zero dynamics is stable. For further details and implications of the notion of *vector relative* degree, the reader is refered to Isidori [9].

Definition A.6. A system of the form $\dot{x} = f(x, u)$; $z = h(x)$, with equilibrium state $\bar{x}$, and corresponding equilibrium input and output values, given by $(x, u, z) = (\bar{x}, \bar{u}, \bar{z})$, is said to be *locally equilibrium state detectable* if there exists a neighbourhood, χ, of $\bar{x}$, such that for all initial states $x \in \chi$, the motions of the system $\dot{\xi} = f(\xi, \bar{u})$, with $\xi(t_0) = x$, which are restricted to the manifold $Z = \{\xi: h(\xi) = \bar{z}\}$, for all $t \geq 0$, locally converge to the equilibrium point, $\bar{x}$. If the neighbourhood χ is all of the state space, then the system is said to be *globally equilibrium state detectable*. Similarly, a system is said to be *locally equilibrium state observable* if there exists a neighbourhood χ of $\bar{x}$, such that for all $x \in \chi$, the motions of the system $\dot{\xi} = f(\xi, \bar{u})$, with $\xi(t_0) = x$, which are restricted to the manifold $Z = \{\xi: h(\xi) = \bar{z}\}$ are the trivial motions, $\xi = \bar{x}$, for all $t \geq 0$. If χ is the whole state space then the system is said to be *globally equilibrium state observable*.

The equilibrium state detectability property is intimately connected with the possibilities of regulation by means of *output feedback*, in place of state feedback (see [3]).