

Application of Nonlinear Time–Scaling for Robust Controller Design of Reaction Systems

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Entia non sunt multiplicanda praeter necessitatem
William of Ockham
c. 1280

Abstract

Even though the basic mechanisms of operation of reaction systems are relatively simple the dynamical models obtained from first principles are complex and contain highly uncertain terms. To develop reliable model–based controllers it is therefore necessary to simplify the system dynamics preserving the features which are essential for control. Towards this end, coordinate transformations identifying the states which are dependent/independent of the reactions and flows have been reported in the literature. This has allowed, for instance, the design of observers which are insensitive to the (usually unknown) reaction functions. The main contribution of this paper is to show the utility of *nonlinear state–dependent time–scaling* to simplify the system dynamics, and consequently the controller design. In particular, we show that with time–scaling and an input transformation we can reveal the existence of attractive invariant manifolds, which allows us to reduce the dimension of the system. As an application we study the well–known fourth order baker’s yeast fed–batch fermentation process model, whose essential dynamics is captured by a planar system perturbed by an exponentially decaying term. We then exploit this particular structure to design, with reduced control authority, a nonlinear asymptotically stabilizing control law which is robust with respect to the reaction function.

Key Words: Reactions systems, time–scaling, fed–batch fermentation processes, nonlinear control.

1 Introduction

The concept of reaction systems [?] refers to a wide class of nonlinear dynamical systems that appears in fields such as chemical engineering, biotechnology, ecology, etc. Even though the basic mechanisms of operation are relatively simple the models are usually quite complex and uncertain,

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therefore various transformations that simplify their dynamics have been proposed. In [?] a linear change of coordinates is used to separate –in reaction systems without inlet and outlet streams– the *reaction-variant* states from the *reaction-invariant* ones. This decomposition is very useful – for instance, for observer design– since the reaction functions are poorly known. In [?] (see also [?]) a *nonlinear* change of coordinates is introduced to extend the concept of reaction invariants of [?] to include *flow* invariants for reaction systems with inlet and outlet streams, thus leading to a decomposition of the state evolution into reaction and flow variants/invariants. The inclusion of a nonlinear transformation, besides adding a significant degree of complexity, might destroy the structure of the system, stymieing the physical interpretation of the transformed system states.

As an alternative to the nonlinear change of coordinates of [?], we propose in this paper a *nonlinear state-dependent time-scaling* which achieves the same objectives. Two important features of our time-scaling are 1) it has a clear physical interpretation in terms of the residence time; 2) it is explicitly computable, allowing for its application not just for analysis purposes, but also for observer and controller design. Nonlinear time-scaling has already been used, among other applications, for feedback linearization in [?, ?].

The main contributions of the paper are as follows. First, we combine the well-known linear change of coordinates of [?] with the proposed time-scaling to derive two *normal forms* –applicable to continuous and fed-batch reactors, respectively– that clearly reveal the reactions and flows variants/invariants and the existence of *attractive invariant manifolds*. The latter allows us to reduce the dimension of the system and simplify the controller design. We also show that using these normal forms we can easily design reaction-independent *observers*, which are simpler than the existing ones and have a guaranteed computable convergence rate in all operating regimes. Second, to illustrate the application of time-scaling for controller design we consider the problem of regulation of the well-known fourth order baker’s yeast fed-batch fermentation process model. It is shown that in the new time-scale, besides the unaccessible subspace, an attractive manifold is revealed, which reduces the essential dynamics to a planar system perturbed by an exponentially decaying term. We then exploit this particular structure to design, with reduced control authority, a nonlinear asymptotically stabilizing control law which is robust with respect to the reaction function. Simulation results that illustrate the performance of our controller are also presented.

2 Reaction network and kinetics

Consider a reaction system with R independent reactions involving S components [?], [?]. Two different mechanisms, *reaction kinetics* and *exchange dynamics*, are involved. The overall dynamics result from the S material balance equations for the S species and the continuity equation for the reactor volume as

$$\Sigma_{n,V}^1 : \begin{cases} \dot{n} &= N^T r_n(n, V) V + C_{in} q_{in} - \frac{q_{out}}{V} n \\ \dot{V} &= Q_{in} - q_{out} \end{cases} \quad (1)$$

with nonnegative initial conditions, where n is the S -dimensional vector of quantities of each species, $Q_{in} \triangleq \sum_{j=1}^p (q_{in})_j$, with q_{in} the p -dimensional inlet volumetric flow-rate vector, q_{out} the outlet volumetric flow rate, V the reactor volume (assumed measurable), N the $R \times S$ constant stoichiometric matrix, and r_n the R -dimensional reaction rate vector, which is a function of n and V . C_{in} is the $S \times p$ inlet constant concentration matrix. The control inputs consist, in general, of the input and output volumetric flow rates, but this may change according to the particular application. Similarly, the available measurements will depend on the problem, which will be made explicit in due course. Due to physical considerations, the validity of the model is restricted to trajectories living in the $S + 1$ -dimensional open positive orthant, which we denote as \mathcal{R}_+^{S+1} . This assumption will be made throughout the paper.

Using the fact that $n = Vc$, with c the concentrations, the model (1) can be rewritten as

$$\Sigma_{c,V}^2 : \begin{cases} \dot{c} &= N^T r_c(c, V) + C_{in} \frac{q_{in}}{V} - \frac{Q_{in}}{V} c \\ \dot{V} &= Q_{in} - q_{out} \end{cases} \quad (2)$$

where $r_c(c, V) = r_n(\frac{n}{V}, V)$. Here, and throughout the rest of the paper, we have used $r_{(\cdot)}((\cdot), V)$ to underscore the use of different arguments in the reaction functions. In typical applications the functions $r_{(\cdot)}$ are highly uncertain, hence we do not give at this point any specific structure to them.

3 Normal forms with time–scaling

The aim of this section is to combine the well-known linear change of coordinates of [?] with a time–scaling to derive two normal forms that, besides revealing the reactions and flows variants/invariants, exhibit the existence of an attractive invariant manifold. The first normal form is derived from (1) and is applicable for continuous reactors, while the second one is obtained from (2) and is useful for both continuous and fed–batch systems.

3.1 First normal form

Under the assumption $\sigma = R + p$, where $\sigma \triangleq \text{rank} [N^T, C_{in}]$, it has been shown in [?] that there exists a linear change of coordinates $z = Tn$ of the form

$$\begin{aligned} z_1 &= (N^+)^T (I_s - C_{in} M^T) n \\ z_2 &= M^T n \\ z_3 &= Q^T n \end{aligned} \tag{3}$$

with M, Q constant matrices of suitable dimensions and $(\cdot)^+$ the pseudoinverse, which transforms (1) into

$$\begin{aligned} \dot{z}_1 &= -\frac{q_{out}}{V} z_1 + r_z(z, V) V \\ \dot{z}_2 &= -\frac{q_{out}}{V} z_2 + q_{in} \\ \dot{z}_3 &= -\frac{q_{out}}{V} z_3 \\ \dot{V} &= -\frac{q_{out}}{V} V + Q_{in} \end{aligned}$$

where z_1, z_2 and z_3 are vectors of dimension R, p and $(S - \sigma)$, respectively.¹ (This linear transformation (3) is a slight modification of the one proposed in [?].) Now, to find the states which are reaction and flow invariants, we should eliminate the term $\frac{q_{out}}{V}$ from the equation of z_3 . Towards this end, a nonlinear state transformation is applied in [?]. The simple observation that we make here is that the same objective can be achieved introducing instead the following time–scaling

$$\frac{dt}{d\tau} = \frac{V}{q_{out}} \tag{4}$$

This time–scaling transformation is well defined (that is, $t \rightarrow \infty \Leftrightarrow \tau \rightarrow \infty$) if $\frac{V}{q_{out}}$ is bounded and bounded away from zero. Recalling our standing assumption that V is bounded away from zero, we have that these conditions holds true for continuous reactors—when $q_{out} \geq \epsilon > 0$.

Applying the chain rule, and introducing the notation $(\cdot)' \triangleq \frac{d(\cdot)}{d\tau}$, we obtain our first normal form

$$\Sigma_{z,V}^1 : \begin{cases} z_1' &= -z_1 + r_z(z, V) v_1 \\ z_2' &= -z_2 + v_2 \\ z_3' &= -z_3 \\ V' &= -V + 1_p^T v_2 \end{cases} \tag{5}$$

where 1_p is a p –dimensional vector with all terms 1, and we have defined the new inputs $v_1 \triangleq \frac{V^2}{q_{out}}$, $v_2 \triangleq q_{in} \frac{V}{q_{out}}$. The system is clearly decomposed into *reactions and flows* variants and invariants. For instance, the only reaction variant is z_1 , which is also flow variant. On the other hand, z_3 is a reaction and flow invariant.

From (5) and (3) we immediately have the following property.

¹For $\sigma < R + p$, the same model (4) can be obtained using a different matrix M , see [?].

Proposition 3.1 *The set $\mathcal{M} \triangleq \{Q^T n = 0\}$, with Q as in (3), is an attractive invariant manifold for the dynamics (1). That is, $(n(0), V(0)) \in \mathcal{M} \Rightarrow (n(t), V(t)) \in \mathcal{M}, \forall t \geq 0$. Furthermore, for all $(n(0), V(0)) \in \mathcal{R}_+^{S+1}$ we have $\lim_{t \rightarrow \infty} Q^T n(t) = 0$.*

It is important to notice that the new time variable can be *explicitly* computed on-line as

$$\tau(t) = \int_0^t \frac{Q_{in}}{V} ds - \log V(t) + \log V(0)$$

revealing the dependence of τ on the *residence-time* –a well-understood quantity in reaction systems.

3.2 Second normal form

The normal form derived in the previous subsection is only applicable to continuous reactors. We will now define a second normal form useful also for fed-batch operation. To this end, we use the model (2), to which we can also apply the linear transformation used in (3), that is $z = Tc$, to get

$$\begin{aligned} \dot{z}_1 &= -\frac{Q_{in}}{V} z_1 + r_z(z, V) \\ \dot{z}_2 &= -\frac{Q_{in}}{V} z_2 + \frac{q_{in}}{V} \\ \dot{z}_3 &= -\frac{Q_{in}}{V} z_3 \\ \dot{V} &= -q_{out} + Q_{in} \end{aligned}$$

with z_1, z_2 and z_3 as before. We now use the residence time to define the time-scaling transformation as

$$\frac{dt}{d\tau} = \frac{V}{Q_{in}} \quad (6)$$

which is valid independently of q_{out} , thus is valid for continuous and fed-batch operation modes. This yields our second normal form

$$\Sigma_{z,V}^2 : \begin{cases} z_1' &= -z_1 + r_z(z, V) u_1 \\ z_2' &= -z_2 + u_2 \\ z_3' &= -z_3 \\ V' &= V - \frac{q_{out} V}{Q_{in}} \end{cases} \quad (7)$$

where we have defined the invertible transformations $u_1 \triangleq \frac{V}{Q_{in}}$, $u_2 \triangleq \frac{q_{in}}{Q_{in}}$. Notice that in *fed-batch* operation, when $q_{out} = 0$, the last equation above further reduces to $V' = V$. Also, as in the previous case, we can compute the new time-scale τ .

The normal forms above, although similar in spirit to the ones obtained via a nonlinear state transformation in [?], [?], are simpler and –in the authors opinion– easier to interpret in terms of physical quantities. In particular, our state variables are still linear combinations of the original species and concentrations variables. Also, the nonlinear input coordinate change, which is introduced only to simplify the notation, still preserves its physical interpretation.

3.3 Observer design

In this subsection we show how to reconstruct the state of the system from a subset of measured concentrations. Towards this end, we recall from [?] the relationship

$$n = \begin{bmatrix} n_s \\ n_t \end{bmatrix} = \begin{bmatrix} N_s \\ N_t \end{bmatrix} z_1 + \begin{bmatrix} C_{in,s} \\ C_{in,t} \end{bmatrix} z_2 + \begin{bmatrix} Q_s \\ Q_t \end{bmatrix} z_3$$

where n_s is an S_s -dimensional *measurable* vector, which induces the indicated partitions of the matrices N, C_{in}, Q . Under the assumptions that $S_s \geq R$ and that N_s^T has a unique left pseudoinverse, we have

$$n_t = N_t^T (N_s^+)^T n_s + A_1 z_2 + A_2 z_3 \quad (8)$$

where $A_1 \triangleq C_{in} - N_t^T (N_s^+)^T C_{in,s}$ and $A_2 \triangleq Q_t - N_t^T (N_s^+)^T Q_s$.

We are in position to present the following proposition. The proof, which is carried out in the τ time-scale, follows immediately from (8), the normal forms (5), (7), and the observation that $z_3(\tau) = \exp^{-\tau} z_3(0) \rightarrow 0$. The latter property –which is revealed by the time-scale change– obviates the need to include an estimate of z_3 . Henceforth, the resulting estimator will be simpler than, e.g., the one reported in [?].

Proposition 3.2 *Consider the reaction system (1). Assume*

1. $\sigma = R + p$, where $\sigma \triangleq \text{rank} [N^T, C_{in}]$;
2. $n_s \in \mathcal{R}^{S_s}$, as defined in (8), is measurable;
3. $S_s \geq R$ and N_s^T has a unique left pseudoinverse.

Under these conditions, the estimator (defined in the time-scale t)

$$\hat{n}_t = N_t^T (N_s^+)^T n_s + A_1 \hat{z}_2 \quad (9)$$

$$\dot{\hat{z}}_2 = -\frac{q_{out}}{V} \hat{z}_2 + q_{in} \quad (10)$$

ensures the estimation error converges to zero as

$$\hat{n}_t(t) - n_t(t) = \frac{V(t)}{V(0)} \exp^{-\int_0^t \frac{Q_{in}}{V} ds} [\hat{n}_t(0) - n_t(0)]$$

On the other hand, if instead of (10) we generate the estimate \hat{z}_2 as

$$\dot{\hat{z}}_2 = -\frac{Q_{in}}{V} \hat{z}_2 + \frac{q_{in}}{V}$$

the estimation error satisfies

$$\hat{n}_t(t) - n_t(t) = \exp^{-\int_0^t \frac{Q_{in}}{V} ds} [\hat{n}_t(0) - n_t(0)]$$

□□□

4 Nonlinear control of the baker's yeast fed-batch fermentation process

In this section, we illustrate the use of the time-scaling to design a robust nonlinear controller for a biotechnological reaction system, the aerobic *baker's yeast growth and fermentation process*.

4.1 Process model

The aerobic *baker's yeast* growth and fermentation process consists of three mass balances for biomass (baker's yeast), substrate (glucose) and ethanol concentrations. Many different models have been proposed in the literature to describe this dynamics. In this work, we consider the model of [?], which was studied for control purposes in [?]. In this case, the reactor operates in a *fed-batch* mode and it is assumed that the substrate concentration in the medium is low and thus there is no ethanol production, however an inhibitory substance is present. This leads to the following model with four states

$$\begin{aligned} \dot{c}_1 &= \psi(c_2, c_3) c_1 - c_1 \frac{q_{in}}{V} \\ \dot{c}_2 &= -\frac{1}{k_y} \psi(c_2, c_3) c_1 + (u_2 - c_2) \frac{q_{in}}{V} - k_m c_1 \\ \dot{c}_3 &= \beta_1 c_1 + \beta_2 \psi(c_2, c_3) c_1 - c_3 \frac{q_{in}}{V} \\ \dot{V} &= q_{in} \end{aligned} \quad (11)$$

where c_1, c_2, c_3 are the concentrations [g/l] of microorganisms, substrate and inhibitory substance, respectively; u_2 is the influent substrate concentration [g/l], which in applications is typically set to a constant value; V is the volume of the reactor [l], q_{in} is the feed of substrate [l/h], and $\beta_1, \beta_2, k_y, k_m$ are positive constants. The reaction function ψ is highly uncertain and we would like to design a controller which is insensitive to its particular shape.

4.2 Problem formulation

Following standard engineering practice, we will consider the following scenario:

(A1) The substrate concentration u_2 is set equal to a *constant* u_2^* (i.e., the only control action is q_{in}).

(A2) c_1 and V are the only variables available for *measurement*.

(A3) The reaction function ψ is *unknown* and, for the purposes of the stability analysis, we only assume that it is uniformly bounded, i.e., $|\psi| \leq M$, and it satisfies the inequality

$$\frac{\partial \psi}{\partial c_2}(c_2, c_3) \geq \beta_2 k_y \frac{\partial \psi}{\partial c_3}(c_2, c_3)$$

(A4) The microorganisms growth does not take place if the substrate is absent, that is, $\psi(0, c_3) = 0$.

It is important to underscore the highly demanding –though practically realistic– scenario that we have fixed. The vast majority of the research reported in the control literature assumes knowledge of the reaction function, full state measurement and availability of u_2 as an additional control signal. See, e.g., [?] and references therein. Notice that no prior knowledge, appart from (A3) and (A4), is required for ψ . Furthermore, the technical assumption (A3) is satisfied by the usual reaction functions, e.g., the combination of a Monod law and a product inhibition function proposed in [?]

$$\psi(c_2, c_3) = \mu_m \frac{c_2}{k_s + c_2} \frac{1}{1 + c_3^2} \quad (12)$$

where the term $\frac{1}{1+c_3^2}$ represents the inhibiting effect of the substance c_3 . We will see below that, in spite of these restrictions, we can exploit the systems structure to regulate the process in a satisfactory manner.

The typical *control objective* is to impose on c_1 a desired growth profile, while keeping c_2 below a given value c_{2max} [?, ?]. (The latter restriction ensures the substrate concentration is low and only growth of the yeast occur without formation of ethanol.) We will express the control objective here in terms of the more standard problem of stabilization of an equilibrium (for the system in the new time scale) containing the point of interest (c_1^*, c_2^*) with c_1^* a *given* positive number, and $0 < c_2^* \leq c_{2max}$.

Our last technical assumption –which is needed to ensure the existence of the equilibrium– concerns the prior knowledge of a steady–state operating regime of the reactor. Namely, we need

(A5) Given u_2^*, c_1^* and c_{2max} , a constant *dilution term* Q^* is *known* such that if we fix $\frac{q_{in}}{V}$ to this value the first three equations of (11) admit an equilibrium point at $c^* \triangleq [c_1^*, c_2^*, c_3^*]$ for some $0 < c_2^* \leq c_{2max}$ and some $c_3^* > 0$.

We will show below that Q^* appears as a tuning parameter for our controller which (essentially) determines the rate of convergence. Recalling that the reactor operates in a fed–batch mode we can, in principle, regulate the transient behavior of c_1 with Q^* or shifting the set–point c_1^* . However, as we will see in the simulations below, care should be taken to avoid an overshoot on c_2 .

4.3 Proposed controller

The proposed robust output feedback controller is given in the proposition below. We refer the interested reader to [?] for an alternative *adaptive* control scheme, which assumes the reaction function is given by (12) but with unknown parameters.

Proposition 4.1 *Consider the bakers–yeast–batch fermentation process (11) with positive initial conditions $c(0), V(0)$ and assumptions (A1)–(A5). The nonlinear static output feedback law*

$$q_{in} = \frac{Q^*}{c_1^*} V c_1 \quad (13)$$

ensures global asymptotic stability of the set $\{c = c^\}$, where $0 < c_2^* \leq c_{2_{max}}$ and $c_3^* > 0$. More specifically, $c(t), V(t)$ remains positive for all $t \geq 0$ and $\lim_{t \rightarrow \infty} c(t) = c^*$.*

Proof: We begin by applying to (11) the time scale transformation $\frac{dt}{d\tau} = \frac{V}{q_{in}}$ and change of input coordinates $u_1 \triangleq \frac{V}{q_{in}}$ of our second normal form, to get

$$\begin{aligned} \dot{c}_1 &= -c_1 + \psi(c_2, c_3) c_1 u_1 \\ \dot{c}_2 &= -c_2 - \frac{1}{k_y} \psi(c_2, c_3) c_1 u_1 - k_m c_1 u_1 + u_2^* \\ \dot{c}_3 &= -c_3 + \beta_1 c_1 u_1 + \beta_2 \psi(c_2, c_3) c_1 u_1 \\ \dot{V} &= V \end{aligned} \quad (14)$$

From simple inspection of (14) we can define an *attractive invariant submanifold* of \mathbb{R}_+^3 as

$$\mathcal{M} = \left\{ \phi(c) \triangleq \left(\frac{1}{k_y} - \beta_2 \frac{k_m}{\beta_1} \right) c_1 + c_2 + \frac{k_m}{\beta_1} c_3 = u_2^* \right\}$$

where $c \triangleq [c_1, c_2, c_3]$. This stems from the (easily verifiable) fact that $\phi' = -\phi + u_2^*$. The existence of \mathcal{M} and the structure of (14) motivates the linear change of coordinates $z_1 = c_1$, $z_2 = c_1 + k_y c_2$, and $z_3 = \phi$, which yields

$$\begin{aligned} \dot{z}_1 &= -z_1 + \psi_z(z) z_1 u_1 \\ \dot{z}_2 &= -z_2 + k_y u_2^* - k_y k_m z_1 u_1 \\ \dot{z}_3 &= -z_3 + u_2^* \end{aligned}$$

where $\psi_z(z) \triangleq \psi\left(\frac{1}{k_y}(z_2 - z_1), \beta_2 z_1 - \frac{\beta_1}{k_m k_y} z_2 + \frac{\beta_1}{k_m} z_3\right)$.² Finally, if we define the input transformation $v_1 = z_1 u_1$ we obtain the following *feedforward form*

$$\begin{aligned} \dot{z}_1 &= -z_1 + \psi_z(z) v_1 \\ \dot{z}_2 &= -z_2 + k_y u_2^* - k_y k_m v_1 \\ \dot{z}_3 &= -z_3 + u_2^* \end{aligned} \quad (15)$$

We will now study the equilibria of (15). In view of Assumption (A5), and the fact that time scaling does not affect the equilibria, we have that (15), with $v_1 = v_1^* \triangleq \frac{c_1^*}{Q^*}$, has an equilibrium at the desired operating point. (Assumption (A5) is then tantamount to say that the reaction function ψ is such that the algebraic equation

$$\psi_z(c_1^*, z_2^*, u_2^*)(z_2^* - k_y u_2^*) + k_y k_m c_1^* = 0$$

²Notice that ψ_z depends on the whole vector $z \triangleq [z_1, z_2, z_3]$.

admits a solution $z_2^* = k_y(u_2^* - k_m \frac{c_1^*}{Q^*})$.) We can thus translate the equilibrium to the origin to get

$$\begin{aligned}\tilde{z}'_1 &= -\tilde{z}_1 + [\psi_z(\tilde{z} + z^*) - \psi_z(z^*)]v_1^* + \psi_z(\tilde{z} + z^*)\tilde{v}_1 \\ \tilde{z}'_2 &= -\tilde{z}_2 - k_y k_m \tilde{v}_1 \\ \tilde{z}'_3 &= -\tilde{z}_3\end{aligned}$$

where we have introduced the notation $(\tilde{\cdot}) \triangleq (\cdot) - (\cdot)^*$. The control law (13) in these new coordinates reduces to $v_1 = v_1^*$, thus we obtain in *closed loop* the cascade system

$$\begin{aligned}\tilde{z}'_1 &= -\tilde{z}_1 + [\psi_z(\tilde{z} + z^*) - \psi_z(z^*)]v_1^* \\ \tilde{z}'_2 &= -\tilde{z}_2 \\ \tilde{z}'_3 &= -\tilde{z}_3\end{aligned}\tag{16}$$

It is well known [?] that the cascade system (16) is (globally) asymptotically stable if

(a) All the solutions of (16) are bounded.

(b) The autonomous subsystem

$$\tilde{z}'_1 = -\tilde{z}_1 + \tilde{\psi}_z(\tilde{z}_1)v_1^*\tag{17}$$

where we defined $\tilde{\psi}_z(\tilde{z}_1) \triangleq \psi_z(\tilde{z}_1 + z_1^*, z_2^*, z_3^*) - \psi_z(z_1^*, z_2^*, z_3^*)$, is (globally) asymptotically stable.

Boundedness of \tilde{z}_2, \tilde{z}_3 is, of course, obvious from (16). On the other hand, boundedness of \tilde{z}_1 is established considering the quadratic function $V_1 = \frac{1}{2}\tilde{z}_1^2$, invoking assumption (A3), and bounding the derivative of V_1 as follows

$$\begin{aligned}V_1' &\leq -\tilde{z}_1^2 + |\tilde{z}_1| |\psi_z(\tilde{z} + z^*) - \psi_z(z^*)| |v_1^*| \\ &\leq -\tilde{z}_1^2 + |\tilde{z}_1| (M + |\psi_z(z^*)|) |v_1^*| \\ &\leq -\frac{1}{2}\tilde{z}_1^2 + \frac{1}{2}(M + |\psi_z(z^*)| |v_1^*|)^2\end{aligned}$$

To prove (b) we recall that any continuously differentiable function f can be decomposed as

$$f(x) = f(0) + \left[\int_0^1 \frac{\partial f}{\partial x}(\lambda x) d\lambda \right] x$$

and, noting that $\frac{\partial \tilde{\psi}_z}{\partial \tilde{z}_1} = \frac{\partial \psi_z}{\partial z_1}$, write $\tilde{\psi}_z(\tilde{z}_1)$ as

$$\tilde{\psi}_z(\tilde{z}_1) = \left[\int_0^1 \frac{\partial \psi_z}{\partial z_1}(\lambda \tilde{z}_1 + z_1^*, z_2^*, z_3^*) d\lambda \right] \tilde{z}_1$$

Now, applying the chain rule and the definition of the coordinate changes, it is easy to show that assumption (A3) ensures that $\frac{\partial \psi_z}{\partial z_1} \leq 0$, hence the term in brackets is also negative. Therefore, multiplying by \tilde{z}_1 on both sides of the equation above we conclude that

$$\tilde{z}_1 \tilde{\psi}_z(\tilde{z}_1) \leq 0$$

The proof of (b) is then concluded evaluating V_1' along the trajectories of (17) as

$$V_1' = -\tilde{z}_1^2 + \tilde{z}_1 \tilde{\psi}_z(\tilde{z}_1)v_1^* \leq -\tilde{z}_1^2$$

where we have used the fact that $v_1^* > 0$. Invoking the result of [?] mentioned above, we conclude that the set $\{c = c^*\}$ is globally asymptotically stable.

It only remains to prove that the positive orthant is invariant and is fully contained in the domain of attraction of the set. Let us denote the first three equations of the closed-loop system (11), (13) as $\dot{c}_i = f_i(c)$, $i = 1, 2, 3$. We will now prove that along the axes $c_i = 0$, $i = 1, 2, 3$ the corresponding

functions $f_i(c)$, $i = 1, 2, 3$ are nonnegative, which establishes that the vector field points towards the (closed) positive orthant. For $i = 1$ we have $f_1(c) = c_1[\psi(c_2, c_3) - \frac{Q^*}{c_1^*}c_1]$, which is zero at $c_1 = 0$ and positive for sufficiently small c_1 . Now,

$$f_2(c_1, 0, c_3) = c_1[-\frac{1}{k_y}\psi(0, c_3) + \frac{Q^*}{c_1^*}u_2^* - k_m]$$

which, given the definition of the equilibrium c^* , is positive under assumption (A4). Finally, given that $\beta_1, \beta_2 > 0$, $f_3(c_1, c_2, 0)$ is clearly positive for all c_1, c_2 . This concludes the proof.

□□□

5 Simulation results

In this section we present the simulation results concerning the robust controller described in the previous section. First, we have studied the equilibrium points of the system (11) for the reaction function (12) for constant control. A simple calculation shows that they are described by a cubic equation of the form

$$a_3(\bar{c}_1, u_2^*)\bar{c}_2^3 + a_2(\bar{c}_1, u_2^*)\bar{c}_2^2 + a_1(\bar{c}_1, u_2^*)\bar{c}_2 + a_0(\bar{c}_1, u_2^*) = 0 \quad (18)$$

For the values of $\bar{c}_1 = c_1^*$ and $u_2^* = u_{2c}^*$ considered in [?] and [?], the equation (18) has no positive real roots \bar{c}_2^* , such that $\bar{c}_2^* \leq c_{2max}$ —this reveals an inconsistency of the mathematical model with experimental data, that was quite surprising for us. It is reasonable then to try to assign the equilibrium $\bar{c}_1 = c_1^*$ by changing u_2^* , but our analysis revealed this to be impossible. Consequently, we looked for a new equilibrium point that maximizes the value of \bar{c}_1 , keeping \bar{c}_2 in the region of interest. It can be verified that, as u_2^* ranges in $(0, u_{2c}^*)$, the admissible equilibrium points belong to the set $\mathcal{C} = \{\bar{c}_1, \bar{c}_2 \mid 0 < \bar{c}_1 \leq c_{1max}, 0 < \bar{c}_2 \leq c_{2max}\}$. It can, furthermore, be shown that for the numerical data of [?] and $c_{1max} = 56$ and $c_{2max} = 0.28$, all the points belonging to this set are stable. It is, therefore expected that a simple linear feedback will preserve stability and add some desired robustness properties. This study, as well as additional detail on the present work, may be found in [?].

Given this previous study, we have chosen for our simulations the set–point $(c_1^*, c_2^*) = (56, 0.23)$ with $u_2^* = 125.022$, being $Q^* = 7.613$ the constant *dilution term* corresponding to this equilibrium point. The initial conditions considered are $c_0 = [10 \ 0.001 \ 0 \ 0]^T$, with $V(0) = 10$.

Firstly, in order to justify the assumption (A5), we have simulated the behaviour of the system for several constant values of the dilution term, in particular for $\frac{q_{in}}{V} = Q^*, 1.11Q^*, 1.25Q^*$. Effectively, we have verified that there is an equilibrium point associated to each constant value of $\frac{q_{in}}{V}$. However, the behaviour of c_2 is practically inadmissible, largely exceeding its maximal allowable value.

Secondly, we have simulated the system with the robust control law (13) varying Q^* . The resulting behaviour is shown in Figures 1 and 2. We can see that this parameter (essentially) determines the rate of convergence of our controller (the convergence rate improves if Q^* is higher). However, we observe that care should be taken to avoid an overshoot on c_2 . Note that, in contrast to [?], the only control action is q_{in} and we assume that only c_1 and V are measurable, thus the resulting behaviour, taking into account the constraints mentioned above, is quite satisfactory.

Finally, we present the effect of adding an integral term $-k_i \int_0^t (c_1 - c_1^*)ds$ in the control law (13). The resulting behaviour is shown in Figures 1 and 2, where we have used Q^* corresponding to $(c_1^*, c_2^*) = (56, 0.23)$ and several values of the parameter k_i . We observe that the steady error is smaller. Again, note that care should be taken to regulate c_2 .

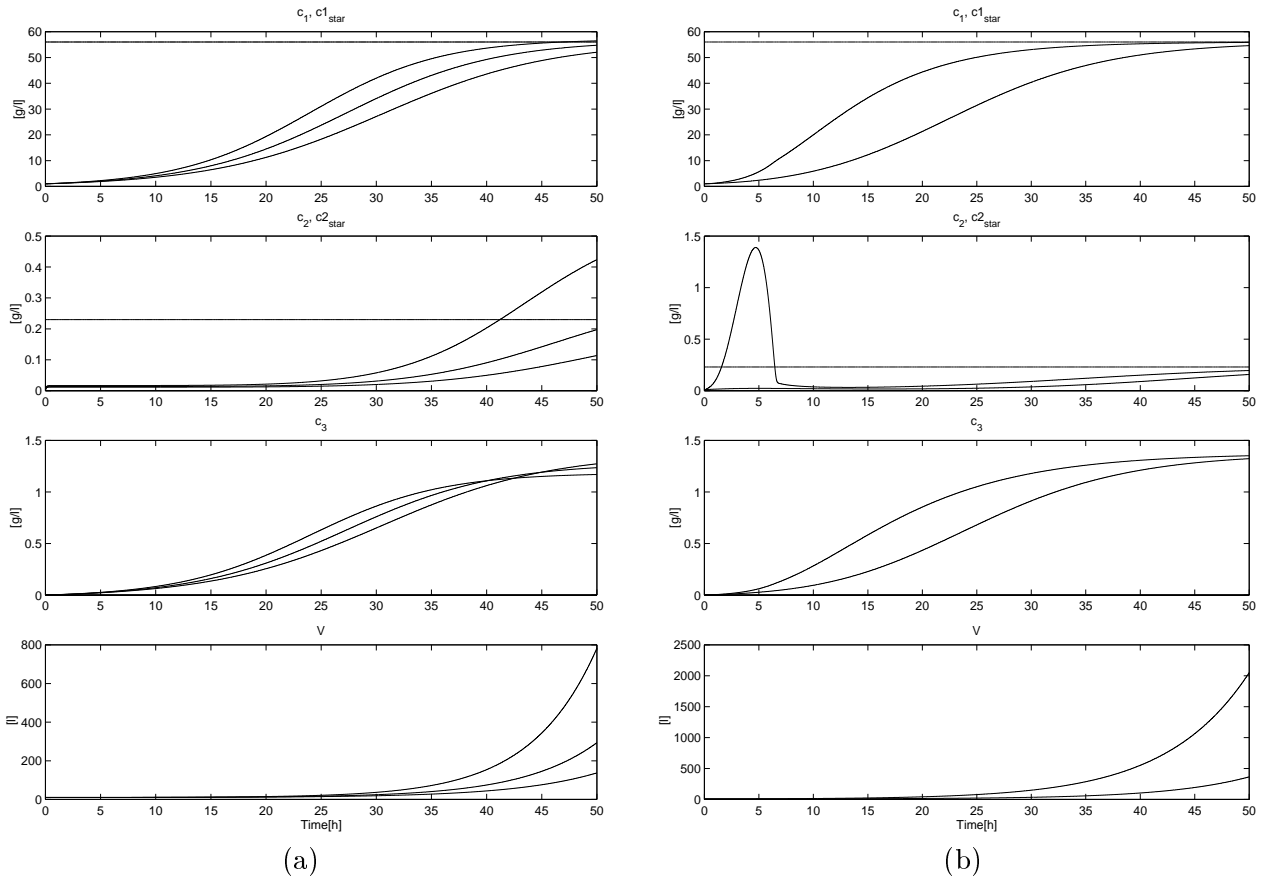


Figure 1: (a) Evolution of the state with the robust control law (13) varying the parameter Q^* , $(Q^*, 1.11Q^*, 1.25Q^*)$. (b) With an integral term, Q^* corresponding to $(c_1^*, c_2^*) = (56, 0.23)$ and varying k_i ($k_i = 10^{-4}, 10^{-3}$).

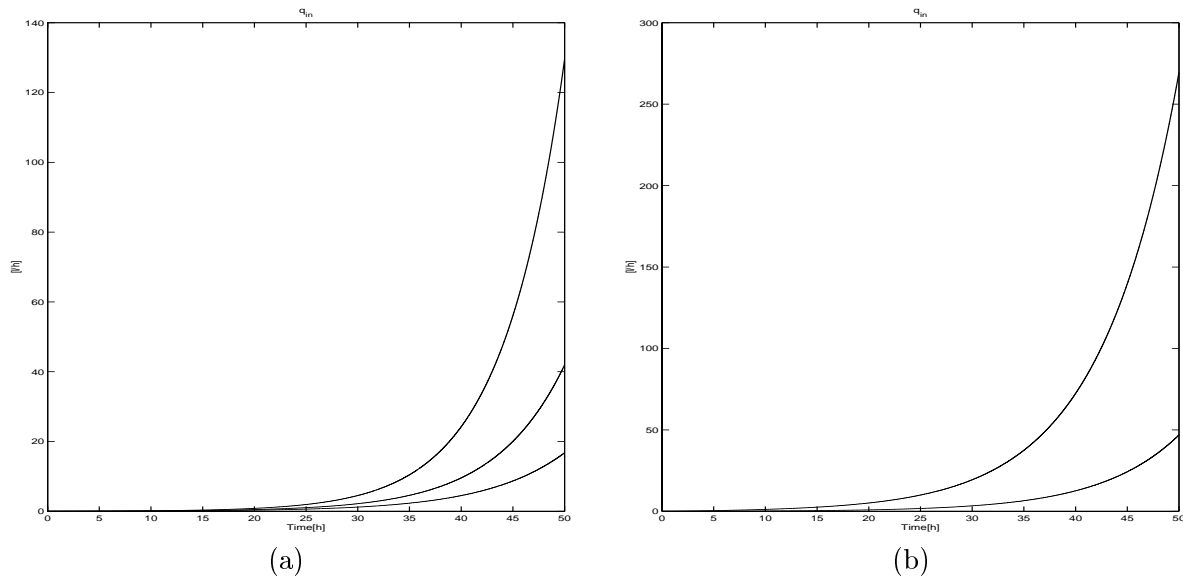


Figure 2: (a) Evolution of the robust control law (13) varying the parameter Q^* , $(Q^*, 1.11Q^*, 1.25Q^*)$. (b) With an integral term, Q^* corresponding to $c^* = (56, 0.23)$ and varying k_i ($k_i = 10^{-4}, 10^{-3}$).

6 Conclusions

The main message of the present work is that the structure of physical systems in general, and reaction systems in particular, can be profitably used for analysis and controller design. In some applications these structural properties are revealed already at the modeling stage. For instance, when using variational modeling for mechanical, electrical or electromechanical systems, see e.g. [?]. See also [?] for a mass balance example where the Hamiltonian structure is suitably exploited. For other classes of systems the first logical step is to apply coordinate changes, which is the approach advocated in [?, ?]. In this paper we have proposed *time-scaling*. This has been used in reaction systems to obtain two, easily interpretable, normal forms which reveal various invariants (with respect to reaction and flow, or asymptotic invariant subspaces) that simplify the analysis and the controller design.

An example of a fed–batch reactor is used to illustrate the main ideas, and a robust scheme with reduced control authority is proposed. Although assumption (A5) can be justified in terms of prior knowledge about the steady state regime, it would be interesting to relax this requirement. This leads to a non–standard adaptive control problem where the equilibrium to be stabilized is unknown. Current investigation is under way to solve this problem.

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