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ON THE PH CONTROL OF A CSTR SYSTEM: AN INVARIANT STABILIZATION APPROACH

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Abstract: We illustrate the relevance of groups of transformations, which qualify as symmetries for the controlled dynamics, in the pH regulation problem for a two species continuously stirred tank reactor (CSTR) system. The existence of a state space symmetry allows to simplify the control design to regulating just one product concentration, while evading well known singularities. A similar property is also established for a set of invariant stabilization errors yielding a different controller design option.

Keywords: pH control, Reactor control, Transformations, Invariance.

1. INTRODUCTION

Symmetries have played a major role in the developments of Physics all along the XX century. Symmetries are commonly found in areas such as: Classical and Celestial Mechanics, Relativity Theory, Quantum Mechanics and Chrystalopraphy. Its mathematical machinery is quite mature and has been the subject of several authoritative books. We mention just a few: the books by Olver (1986, 1995) the book by Marsden (1994) and the book by Bluman and Kumei (1989). Structural aspects of nonlinear affine systems, such as sub-system decomposition, were the object of a rather complete study by Grizzle and Marcus (1985). The notion of symmetry was investigated, in the context of linear dynamic systems, in an article by Fagnani and Willems (1993). Symmetry has recently found renewed interest in nonlinear control systems synthesis problems. In the work of Martín and Rouchon, (1999), applications of symmetries were made to clearly explain the direct and indirect field oriented control methods in in-

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duction motors. In a recent book, containing a contributed chapter by Rouchon and Rudolph (1999), the symmetry-based control techniques were naturally extended to the stabilization, and tracking, of differentially flat systems. In that chapter two examples are presented: the trajectory tracking for a nonholonomic car and the regulation of a two species constant volume chemical reactor. In this article, we approach the nonlinear feedback pH regulation of a Continuously Stirred Tank Reactor (CSTR) system, studied by McAvoy *et al* (1972), by examining the group of symmetries admitted by the normalized representation of its controlled dynamics. We show that the CSTR controlled dynamics admits a simple state symmetry group. The existence of this symmetry implies the possibility of reducing the control problem to the stabilization of just one species. Singularity free stabilizing invariant feedback laws are found by straightfoward linearization. Invariant state stabilization errors can also be identified in terms of diffeomorphic transformations with similar model reduction properties. A feedback controller is also proposed for the simultaneous stabilization of these errors to the origin of coordinates, thus achieving the desired pH regulation. Simulations are carried on a typical CSTR system subject to control input saturations. The article is organized as follows: Section 2 describes the CSTR system and defines the pH regulation problem. In that section, we also find a convenient *normalized* model of the chemical process. The normalized model is easily shown to admit a symmetry with respect to 180 degree rotations of the state plane, followed by a fixed translation. We also identify a diffeomorphic transformation, relevant to the system stabilization task, that qualifies as an equilibrium stabilization error vector. The two independent errors are shown to satisfy exactly the same controlled differential equation, thus simplifying the controller design problem to a one dimensional problem. Section 3 presents computer simulations evaluating the performance of the prescribed feedback controllers. The last section is devoted to conclusions and suggestions for further research. A summary of symmetry and invariance is provided for background purposes. The exposition is directly taken from Rouchon and Rudolph (1999).

2. AN INVARIANT STABILIZATION APPROACH TO PH REGULATION IN A CSTR

2.1 *A brief introduction to symmetry and invariance*

We give here an elementary introduction to the concept of *symmetry* and *invariance*. We follow, very closely, the terse presentation given by Rouchon and Rudolph (1999) where the reader is referred for further details. Consider a controlled system of the form, $\dot{z} = f(z, v)$, with the state, $z \in M$ and $dim\ M = n$, and control input, $v \in R$. Let G be a finite order *local group* of transformations on $M \times R$, which takes the variables (z, v) into (ω, ϑ), according to:

$$\omega = \varphi_g(z), \quad \vartheta = \psi_g(z, v), \quad g \in G$$

We say that the system $\dot{z} = f(z, v)$ admits G as a local *symmetry group* if and only if, for each $g \in G$ there exists a regular static feedback $\vartheta = \psi_g(z, v)$ such that

$$\dot{\omega} = f(\omega, \vartheta)$$

i.e. the system equations remain invariant under the transformation, modulo regular static feedback. If $\vartheta = \psi_g(z, v) = v$ for all $g \in G$, the system is said to admit a *state space symmetry* group. We let, $(\overline{z}, \overline{v})$, denote the constant equilibrium values of the system, i.e. $f(\overline{z}, \overline{v}) = 0$. An *invariant static state feedback* is a mapping $k : M \times M \times R$, defined by

$$v = k(z, \overline{z}, \overline{v})$$

such that for all $g \in G$ the following invariance condition holds:

$$k(\varphi_g(z), \varphi_g(\overline{z}), \psi(\overline{z}, \overline{v})) = \psi_g(z, k(z, \overline{z}, \overline{v}))$$

An invariant static state feedback is said to be *globally (resp. locally) asymptotically stabilizing* at $(\overline{z}, \overline{v})$, if globally (resp. locally) in $M \times R$, one has that: $(z, v) \rightarrow (\overline{z}, \overline{v})$ as $t \rightarrow \infty$. A global (resp. local) invariant state error with respect to the point $(\overline{z}, \overline{v}) \in M \times R$ is a *set of invariants* of G

$$e(z, \overline{z}, \overline{v}) = (e_1(z, \overline{z}, \overline{v}), \ldots, e_n(z, \overline{z}, \overline{v}))$$

such that $(e_1, \ldots, e_n)$ is a local (resp. global) diffeomorphism on M and $e(\overline{z}, \overline{z}, \overline{v}) = 0$.

2.2 *The reactor dynamics*

Figure 1 shows a CSTR system, taken from McAvoy *et al* (1972), where two input feeds are considered: The feed F_1 is the sodium hydroxide, (NaOH), volumetric feed, considered as the control input, which is also assumed to exhibit a constant input concentration C_1, while the second feed, F_2, is the constant input flow of acetic acid (HAC) which is also assumed to have a constant input concentration, given by C_2. The volume V of the tank is also assumed to be constant. A dynamic model for the pH regulation in the tank is given by the following set of differential equations:

$$
\begin{aligned}
V\frac{d}{dt}x_1 &= -F_2 x_1 + u(C_1 - x_1) \\
V\frac{d}{dt}x_2 &= F_2(C_2 - x_2) - u x_2
\end{aligned} \tag{1}
$$

where x_1 is the sodium concentration, x_2 is the combined concentration of acetic acid and the acetate ion $[AC^-]$ concentration. The control input u is the NaOH volumetric feed. We denote by y the hydrogen ion, $[H^+]$, concentration at the output of the reactor, which is to be regulated. The pH of the output product is given by,

$$
\mathrm{pH} = -\log_{10}(y) \tag{2}
$$

where y is represented by the real solution of the following algebraic equation,

$$
\begin{aligned}
& y^3 + (K_a + x_2)y^2 + [K_a(x_2 - x_1) - K_w]\, y \\
& -K_a K_w = 0
\end{aligned} \tag{3}
$$

with K_a and K_w being known constants representing, respectively, the acetic acid equilibrium constant and the water equilibrium constant, respectively.

2.3 *Problem formulation*

Suppose it is desired to regulate the pH towards a desired equilibrium value, given by, $\overline{\mathrm{pH}}$. The system equations (1) reveal that the equilibria for x_1 and x_2, denoted by $\overline{x}_1$ and $\overline{x}_2$, are related by:

$$
C_2\overline{x}_1 + C_1\overline{x}_2 = C_1 C_2 \tag{4}
$$

From the output equations (2), (3) and the equilibrium relation (4), it follows that it is possible to parameterize the equilibria for x_1 and x_2, solely in terms of $\overline{y} = 10^{-\overline{\mathrm{pH}}}$, as follows,

$$
\begin{aligned}
\overline{x}_2 &= \frac{C_2}{C_1}(C_1 - \overline{x}_1) \\
&= -\frac{(\overline{y} + \sqrt{K_w})(\overline{y} - \sqrt{K_w})(\overline{y} + K_a) - K_a\overline{y}C_1}{\overline{y}[\overline{y} + K_a\,(1 + C_1/C_2)]}
\end{aligned} \tag{5}
$$

The pH regulation problem is, therefore, equivalent to the stabilization of (x_1, x_2) towards its desired equilibrium value $(\overline{x}_1, \overline{x}_2)$, computed in accordance with (5). For this reason, from now on, we concentrate on the state regulation task.

2.4 *Normalization of the reactor state dynamics*

The following state, input, and time scaling transformation,

$$
z_1 = \frac{x_1}{C_1}, \quad z_2 = \frac{x_2}{C_3}, \quad v = \frac{u}{F_2}, \quad \tau = \left(\frac{F_2}{V}\right) t
$$

yields the following, appealing, *normalized* representation of the pH regulation process dynamics,

$$
\begin{aligned}
\dot{z}_1 &= -z_1 + v(1 - z_1) \\
\dot{z}_2 &= (1 - z_2) - v z_2
\end{aligned} \tag{6}
$$

where now the "dot " notation, abusively, stands for derivation with respect to the scaled time τ. For constant, positive, values of the normalized input, $v = \overline{v}$, the state of the system has the following, strictly positive, control parameterized equilibria,

$$
\overline{z}_1 = \frac{\overline{v}}{1 + \overline{v}}, \quad \overline{z}_2 = \frac{1}{1 + \overline{v}}, \implies \quad \overline{z}_1 + \overline{z}_2 = 1
$$

It can be shown, with very little effort, that the state variables z_1 and z_2 constitute, each one of them, *minimum phase outputs*. This fact is quite helpful since controlling one of these "outputs" towards a desired constant equilibrium point, automatically makes the system regulate the second state variable towards its own equilibrium point. Indeed, suppose $z_1 = \overline{z}_1$ is constant, the *zero dynamics*, corresponding to the output z_1, is given by

$$
\begin{aligned}
\dot{z}_2 &= -\left(\frac{1}{1 - \overline{z}_1}\right)(z_2 - 1 + \overline{z}_1) \\
&= -\left(\frac{1}{\overline{z}_2}\right)(z_2 - 1 + \overline{z}_1)
\end{aligned}
$$

whose trajectories are asymptotically stable towards $\overline{z}_2 = 1 - \overline{z}_1$. A similar procedure shows that z_2 is also a minimum phase output.

2.5 *A symmetry for the normalized system*

The search for a symmetry can be approached just by considering its definition. We have to find a Lie group of transformations, $\omega = \varphi(z) = (\varphi_1, \varphi_2)$, of the state coordinates $z = (z_1, z_2)$, such that, modulo regular state feedback (i.e. state dependent input coordinate transformation), the system equations remain exactly the same as before, but now, in terms of the transformed state and input variables. It turns out that, in this particular case, the system admits a state space symmetry We, thus, obtain, for φ, the following set of partial differential equations:

$$
\begin{aligned}
-z_1 \frac{\partial \varphi_1}{\partial z_1} + (1 - z_2)\frac{\partial \varphi_1}{\partial z_2} &= -\varphi_1 \\
(1 - z_1)\frac{\partial \varphi_1}{\partial z_1} - z_2 \frac{\partial \varphi_1}{\partial z_2} &= 1 - \varphi_1 \\
-z_1 \frac{\partial \varphi_2}{\partial z_1} + (1 - z_2)\frac{\partial \varphi_2}{\partial z_2} &= 1 - \varphi_2 \\
(1 - z_1)\frac{\partial \varphi_2}{\partial z_1} - z_2 \frac{\partial \varphi_2}{\partial z_2} &= -\varphi_2
\end{aligned} \tag{7}
$$

We readily obtain, by straightforward inspection, that a possible solution of the system (7), is given by the following simple diffeomorphic state coordinate transformation,

$$\varphi_1 = \omega_1 = 1 - z_2, \quad \varphi_2 = \omega_2 = 1 - z_1 \tag{8}$$

It is straightforward to verify that this non singular transformation leaves the controlled system equations (6) *invariant*, without any need for further feedback. The transformed differential equations, written in terms of the new variables, ω_1 and ω_2, are, thus, given by

$$
\begin{aligned}
\dot{\omega}_1 &= -\omega_1 + v(1 - \omega_1) \\
\dot{\omega}_2 &= (1 - \omega_2) - v\omega_2
\end{aligned} \tag{9}
$$

The existence of the symmetry (8) readily reveals that the pH feedback regulation problem can be immediately reduced to control just one dynamic equation. Indeed, consider the diffeomorphism (which is not a symmetry) given by,

$$\varpi_1 = 1 - z_2, \quad \varpi_2 = z_1, \quad \longrightarrow \quad \overline{\varpi}_1 = \overline{\varpi}_2$$

we obtain,

$$
\begin{aligned}
\dot{\varpi}_1 &= -\varpi_1 + v(1 - \varpi_1) \\
\dot{\varpi}_2 &= -\varpi_2 + v(1 - \varpi_2)
\end{aligned} \tag{10}
$$

which are identical controlled differential equations, possibly starting from different initial conditions but having the same equilibrium. Thus, given a desired equilibrium $z_1 = \overline{z}_1 = \overline{\varpi}_2$, a simple linearizing controller, such as,

$$v = \frac{\varpi_2 - K(\varpi_2 - \overline{\varpi}_2)}{1 - \varpi_2} = \frac{z_1 - K(z_1 - \overline{z}_1)}{1 - z_1}$$

with $K > 0$, asymptotically exponentially stabilizes $z_1 \to \overline{z}_1$, and $z_2 \to 1 - \overline{z}_1 = \overline{z}_2$. With respect to the symmetry (8), the linearizing feedbacks,

$$
\begin{aligned}
v = k_1(z, \overline{z}) &= \frac{z_1 - K(z_1 - \overline{z}_1)}{1 - z_1}, \\
v = k_2(z, \overline{z}) &= \frac{1 - z_2 + K(z_2 - \overline{z}_2)}{z_2}
\end{aligned}
$$

satisfy the invariance property $k_i(\omega, \overline{w}) = k_i(z, \overline{z})$. Evidently they constitute local *invariant asymptotically stabilizing feedbacks* at $(\overline{z}_1, \overline{z}_2)$.

2.6 *Invariant stabilization errors*

Consider the following invariant error vector $e(z, \overline{z})$, locally defined in $(0,1) \times (0,1) \subset R^2$, as

$$e_1 = \frac{1 - z_2}{z_2} - \overline{v}, \quad e_2 = \frac{z_1}{1 - z_1} - \overline{v} \tag{11}$$

They evidently constitute a local diffeomorphic transformation of the state space of coordinates, $z = (z_1, z_2)$ which satisfies: 1) $e(\omega, \overline{\omega}) = e(z, \overline{z})$, 2) $e(\overline{z}, \overline{z}) = 0$ and 3) it takes the normalized system (6) to

$$
\begin{aligned}
\dot{e}_1 &= -(e_1 + \overline{v}) - (e_1 + \overline{v})^2 + v(1 + e_1 + \overline{v}) \\
\dot{e}_2 &= -(e_2 + \overline{v}) - (e_2 + \overline{v})^2 + v(1 + e_2 + \overline{v})
\end{aligned} \tag{12}
$$

i.e., both errors satisfy exactly the same controlled differential equation and the feedback regulation problem reduces to control just one of these errors to zero. Notice that if, for any $K > 0$, we specify the following feedback controller,

$$v = -\frac{K e_1}{1 + e_1 + \overline{v}} + \overline{v} + e_1 \tag{13}$$

one obtains an asymptotically stable error dynamics regulated by $\dot{e}_1 = -K e_1$. The same feedback, written in terms of e_2, yields $\dot{e}_2 = -K e_2$.

2.7 *A remark on the flatness of the normalized system*

The system exhibits a *flat output* (see the article by Fliess *et al*, 1995) given by the following quantity:

$$R = \frac{z_2}{1 - z_1},$$

whose equilibrium value is readily found to be, $\overline{R} = 1$. It is easy to see that all the normalized system state variables and the normalized control input can all be differentially parameterized in terms of the flat output, R.

$$z_1 = \frac{1 - R - \dot{R}}{1 - R}, \; z_2 = \frac{\dot{R}R}{1 - R}, \; v = -1 - \frac{\ddot{R}}{\dot{R}}$$

The parameterization is clearly singular around the constant equilibrium points of the system. Any controller directly designed on the basis of the differential flatness of the system, will have to resolve these singularities by *ad hoc* techniques. The controllers designed above do not exhibit any of these singularities.

3. SIMULATION RESULTS

Simulations were performed on a CSTR system with the following parameters:

$$V = 1000 \text{ [lt]}, \quad F_2 = 515 \text{ [lt/min]},$$

$$C_1 = 0.3178 \text{ [mol/lt]}, \quad C_2 = 0.0\,5 \text{ [mol/lt]},$$

$$K_w = 10^{-14}, \quad K_a = 1.8 \times 10^{-5}$$

It was desired to regulate the pH, from an arbitrary initial value towards the value of 9, i.e.

$$\overline{\text{pH}} = 9 \implies \overline{y} = 10^{-9}$$

The prescribed control objective implied that the equilibrium values for the original state variables, x_1, x_2, are given by:

$$\overline{x}_1 = 0.0432 \text{ [mol/lt]}, \quad \overline{x}_2 = 0.0432 \text{ [mol/lt]}$$

with the corresponding equilibrium value for the control input u given by

$$\overline{u} = 81 \text{ [lt/min]}$$

In order to give a realistic feature to the control scheme, we implemented a controller which could only take positive values in the closed interval, $u \in [0, 150]$ [lt/min]. Figure 2 depicts the performance of the feedback controller given by equation (2.5). The concentrations of the original state variables x_1 and x_2 are shown to converge towards their common desired equilibrium value. The control input is initially saturated at the lower bound. In spite of the lack of feedback during the initial stage, the controller stabilizes the system towards the desired equilibrium. Figure 3 depicts the performance of the feedback controller given by equation (13). The concentrations of the original state variables x_1 and x_2 are shown to also converge towards their common desired equilibrium value. The control input is initially saturated at the upper bound.

4. CONCLUSIONS

In this article we have provided and instance of application of symmetry groups for the simplification of a nonlinear control problem. The treated example corresponded to the pH control of a two species CSTR system. The normalized model of the system was shown to exhibit a state space symmetry which immediately revealed the redundancy of the state model for feedback controller design purposes. A local diffeomorphism, which is relevant to the equilibrium stabilization problem, was shown to exhibit the same model simplifying properties encountered by symmetry considerations. Any of the components of the diffeomorphism qualifies also as an invariant error for the non-redundant system. The derived controllers performed rather well in spite of realistic saturation limits that were imposed on the control input implementation. The notion of symmetry seems to have direct relevance in sliding mode control, Lyapunov stability theory and other controller design methodologies. These topics deserve attention for further research.

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FIGURES

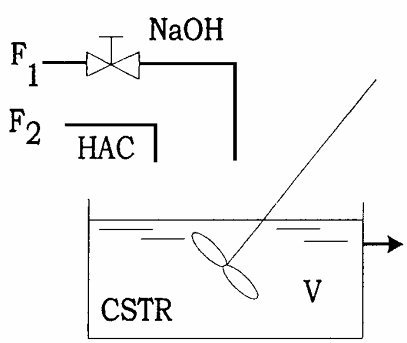

Fig. 1. Continuously Stirred Tank Reactor System.

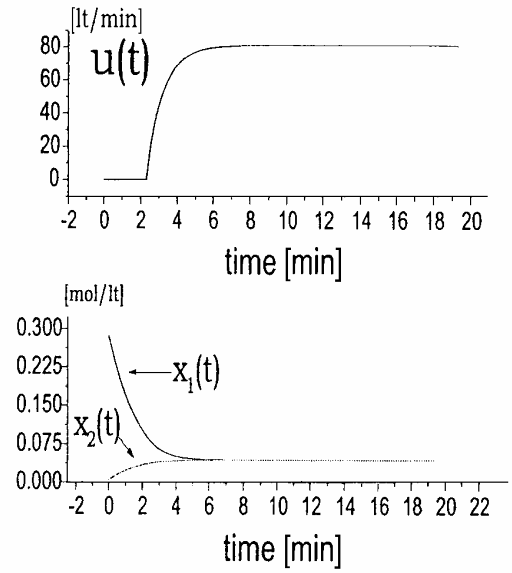

Fig. 2. Control and state responses of CSTR system, linearizing control.

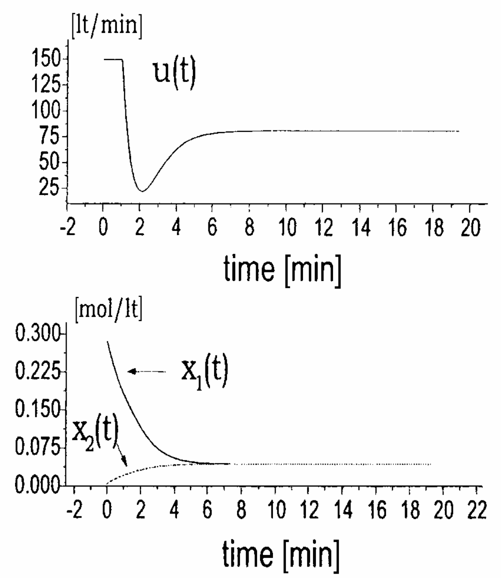

Fig. 3. Control and state responses of CSTR system, invariant error control.