Vibrational control and flatness of chemical reactors

Pierre Rouchon
Ecole des Mines de Paris, Centre Automatique et Systmes
60, Bd Saint Michel, 75272 Paris Cdex 06
Email: rouchon@cas.ensmp.fr

Abstract

Forces oscillations introduced in the input flow rate of non flat continuous stirred-tank reactors (CSTR with 3 independent species) are shown to result in an averaged flat system with linearizing output independent of the special form of the kinetics laws.

1 Introduction

In [4, 3] the stabilization of a chemical reactor around an unstable operating point is investigated: open-loop oscillations of the input flow rate yields a stable averaged behavior. In [5, 6], experimental results demonstrate the practical interest of such control techniques.

For mechanical system, these stabilization techniques are well known since the work of Kapitsa [10]: the unstable position of an inverted pendulum is stabilized via fast oscillations of its suspension point (see also [2] for closely computations). In [7], we have shown how such oscillatory control can be fully exploited for the Kapitsa pendulum: this non flat system is approximated by an averaged flat one for which standard motion planning and exponential tracking techniques can be used.

In this paper, we propose similar results for a class of non flat chemical reactors involving three independents species and one control (the input flow rate). This class is more complex that the one considered in [5, 6] (two species and one control). We show here that the averaged flat output admits a clear physical interpretation and is independent of the precise form of the kinetics an thermodynamics laws.

2 Reactor model

The mass and energy balances of a continuous stirred tank reactor, with constant volume and pressure, involving three independent species (components A and B, h the enthalpy), admit the following structure:

$$\frac{d}{dt}\begin{pmatrix} c_A \\ c_B \\ h \end{pmatrix} = D\begin{pmatrix} c_{A_{in}} - c_A \\ c_{B_{in}} - c_B \\ h_{in} - h \end{pmatrix} + \begin{pmatrix} r_1(h, c_A, c_B) \\ r_2(h, c_A, c_B) \\ r_3(h, c_A, c_B) \end{pmatrix} \tag{1}$$

where D, the control, is the dilution rate, $c_{A_{in}}$, $c_{B_{in}}$ and h_{in} are the feed compositions and enthalpy (perturbations), the r_i's are smooth functions of their arguments depending on the kinetics and thermodynamics models. The state (c_A, c_B, h) corresponds to the concentration of A, B and to the volume enthalpy in the reactor. When enthalpies depend linearly on the temperature T, we recover the standard equations.

It is clear that, in general, this model is not differentially flat: it admits one control; thus flatness is equivalent to static feedback linearization and the necessary and sufficient conditions [9] give to a negative answer, in general.

3 Pulse control of D

Consider, as in [5, 6], a pulse control for D

$$D = D_0 + \frac{D_1}{\varepsilon}\,\sigma(t/\varepsilon) \tag{2}$$

where ε is a small positive parameter, D_0 and D_1 are new controls and σ is a 1-periodic function, not necessary smooth but bounded and integrable with $\int_0^1 \sigma(s)ds = 0$. Thus σ can be seen as the derivative of a periodic function, Σ: $\sigma = \Sigma'$; Σ can be always chosen such that $\int_0^1 \Sigma(s)ds = 0$.

Set

$$\xi = \begin{pmatrix} c_{A_{in}} - c_A \\ c_{B_{in}} - c_B \\ h_{in} - h \end{pmatrix}, \quad \xi_{in} = \begin{pmatrix} c_{A_{in}} \\ c_{B_{in}} \\ h_{in} \end{pmatrix}.$$

With (2), the reactor equations (1) become

$$\dot{\xi} = \dot{\xi}_{in} - \left(D_0 + \frac{D_1}{\varepsilon}\,\sigma(t/\varepsilon)\right)\,\xi - R(\xi)$$

where $R = (r_1, r_2, r_3)'$.

In these coordinates, the system is not in standard form for averaging [8, 14, 1] (terms involving $1/\varepsilon$). A change of variables, depending on t/ε, is required.

As shown in [4, 3], this corresponds to straighten the vector fields $\xi \mapsto -\xi$. The goal is to cancel the terms depending on $1/\varepsilon$. We have

$$\dot{\xi} + \frac{d}{dt}(D_1\Sigma(t/\varepsilon)) \;\; \xi = \dot{\xi}_{in} - D_0\xi + \dot{D}_1\Sigma(t/\varepsilon)\; \xi - R(\xi).$$

Set $\xi = \exp(-D_1\Sigma(t/\varepsilon))\; \zeta$. Then

$$\dot{\xi} = -\frac{d}{dt}(D_1\Sigma(t/\varepsilon))\; \xi + \exp(-D_1\Sigma(t/\varepsilon))\; \dot{\zeta}.$$

Thus the ζ-coordinates remove the terms in $1/\varepsilon$:

$$\begin{array}{c}\dot{\zeta} = \exp(D_1\Sigma(t/\varepsilon))\; \dot{\xi}_{in} - (D_0 - \dot{D}_1\Sigma(t/\varepsilon))\; \zeta \\ - \exp(D_1\Sigma(t/\varepsilon))\; R(\exp(-D_1\Sigma(t/\varepsilon))\zeta).\end{array}$$

Now the system is in standard form: the averaged system is then

$$\begin{array}{c}\dot{\bar{\zeta}} = \overline{\exp(D_1\Sigma(t/\varepsilon))}\; \dot{\xi}_{in} - (D_0 - \dot{D}_1\overline{\Sigma})\; \bar{\zeta} \\ -\overline{\exp(D_1\Sigma(t/\varepsilon))\; R(\exp(-D_1\Sigma(t/\varepsilon))\zeta)}\end{array}$$

where $\overline{H(t/\varepsilon,\zeta)} = \int_0^1 H(s,\zeta)ds$ for any function H. But $\overline{\Sigma} = 0$. Pulling back into the original coordinates $\bar{\xi} = \overline{\exp(-D_1\Sigma)}\; \bar{\zeta}$, we obtain finally the following averaged system

$$\dot{\bar{\xi}} = E(D_1)\; \dot{\xi}_{in} - D_0\; \bar{\xi} - F(D_1, \bar{\xi})$$

with

$$\begin{array}{c}E(D_1) = \\ \left(\int_0^1 \exp(-D_1\Sigma(s))\; ds\right)\left(\int_0^1 \exp(D_1\Sigma(s))\; ds\right)\end{array}$$

and

$$F(D_1,\bar{\xi}) = \int_0^1 \left(\exp(D_1\Sigma(s))\; R\left(\frac{\exp(-D_1\Sigma(s))\; \bar{\xi}}{\overline{\exp(-D_1\Sigma)}}\right)\right)\; ds.$$

4 The averaged system is flat

The above computations prove that the averaged concentrations $\bar{c}_A$, $\bar{c}_B$ and enthalpy $\bar{h}$ obey (at a first order in ε) the following dynamics with two controls D_0 and D_1:

$$\begin{array}{c}\dfrac{d}{dt}\begin{pmatrix}\bar{c}_A\\ \bar{c}_B\\ \bar{h}\end{pmatrix} = D_0\begin{pmatrix}c_{A_{in}} - \bar{c}_A\\ c_{B_{in}} - \bar{c}_B\\ h_{in} - \bar{h}\end{pmatrix} \\ +(1 - E(D_1))\; \dfrac{d}{dt}\begin{pmatrix}c_{A_{in}}\\ c_{B_{in}}\\ h_{in}\end{pmatrix} \\ +\begin{pmatrix}\rho_1(D_1,\bar{h},\bar{c}_A,\bar{c}_B)\\ \rho_2(D_1,\bar{h},\bar{c}_A,\bar{c}_B)\\ \rho_3(D_1,\bar{h},\bar{c}_A,\bar{c}_B)\end{pmatrix}\end{array} \tag{3}$$

where

$$\rho_i(D_1, \bar{h}, \bar{c}_A, \bar{c}_B) = \int_0^1 (\exp(D_1\Sigma(s)) \ \ldots... r_i\left(\frac{\exp(-D_1\Sigma(s))\ \bar{h},}{\overline{\exp(-D_1\Sigma)}}, \frac{\exp(-D_1\Sigma(s))\ \bar{c}_A,}{\overline{\exp(-D_1\Sigma)}}, \frac{\exp(-D_1\Sigma(s))\ \bar{c}_B,}{\overline{\exp(-D_1\Sigma)}}, \right)\right) ds$$

with $\overline{\exp(-D_1\Sigma)} = \int_0^1 \exp(-D_1\Sigma(s))\ ds$.

Proposition *For generic functions r_i and Σ, the averaged system (3), is flat with*

$$y_1 = \frac{c_{A_{in}} - \bar{c}_A}{h_{in} - \bar{h}} \quad \textit{and} \quad y_2 = \frac{c_{B_{in}} - \bar{c}_B}{h_{in} - \bar{h}}$$

as flat output.

A simple computation shows that $\dot{y}_1$ and $\dot{y}_2$ do not depend on D_0. Thus, generically, the averaged state and the control D_1 are functions of $y = (y_1, y_2)$ and $\dot{y}$. An additional derivation yields D_0 has a function of $(y, \dot{y}, \ddot{y})$.

It is interesting to notice that, as in [13] ,the flat output is independent of the special form of the kinetics and thermodynamics laws.

5 Conclusion

In future publications, simulations will be performed. They will correspond to the reaction scheme of [11, 12] taking place in an adiabatic vessel. This will show that the use of such control technic can eliminate the cooling system and consequently could yield to substantial savings in energy.

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