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Geometric-dissipative control of exothermic continuous reactors

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Abstract: The problem of robustly stabilizing through output-feedback control an open-loop unstable exothermic continuous reactor with temperature measurement is addressed. The combination of advanced geometric control and classical mechanics methods yields: (i) solvability of the detailed model-based nonlinear output-feedback problem in terms of passivity, observability and dissipativity, (ii) open-loop energy and closed-loop Lyapunov functions in analytic form, and (iii) the tradeoff between response speed, robustness, and control effort. On the basis of simplified model tailored according to the passivity-observability-dissipativity structure, the advanced geometric observer-based nonlinear controller is realized with an industrial-like PID controller. The methodology is illustrated with numerical simulations.

Keywords: Chemical reactor, output-feedback control, PID control, Lyapunov function, geometric control, passive control, dissipative control, mechanical control.

1. INTRODUCTION

Amundson and Aris (AA) studied the open loop (OL) dynamics and the closed-loop (CL) behavior with linear P, PI and PID control of a two-state continuous exothermic jacketed single-component chemical reactor (Aris and Amundson; 1959a-c), by combining reactor engineering and global dynamics insight, local stability analysis with analytic formula, and global dynamics with analog simulation. The reactor has a rather reach, simple and complex, dynamical nonlinear behavior over its parameter space (Van Heerden, 1953; Uppal et al, 1974), and has become a benchmark for advanced and conventional control development. The related literature is abundant and disperse (in few reactor *per se* studies and in many ones with the reactor as application example of general-purpose control designs), and here it suffices to mention that, in spite of significant advances with valuable insight, there are still open problems, among them are two addressed in the present study: (i) the first principle-based construction of control Lyapunov functions, and (ii) the rigorous connection between advanced nonlinear and industrial linear control approaches.

Here, the problem of stabilizing with temperature-driven output-feedback (OF) control AA's reactor at an unstable-nonunique steady-state (SS) is addressed, with emphasis on: (i) the trade-off between response speed, robustness, and control effort, and (ii) the formal connection between advanced nonlinear (passive and dissipative) and industrial (PID) control.

The points of departure are: (i) the nonlocal saturated robust nonlinear state-feedback (NLSF) stabilizing control (Alvarez et al, 1991; El-Farra and Christofides,2003), (ii) the observer-based (Alvarez and Fernández, 2009) geometric passive NLOF geometric control and its connection with linear PI control (Alvarez Ramírez et al, 2002; Gonzalez and Alvarez, 2005; Schaum et al., 2015), (iii) global motion observability (Diaz-Salgado et al. 2012, Moreno and Alvarez, 2015), (iv) classic mechanics (Corben and Stehle, 1960), and (v) thermodynamics-based constructions of Lyapunov functions (Ydstie, 2002; Favache et al, 2011) for control design via dissipation for abstract (Solis-Down, 2013) and electro-mechanical systems (Ortega et al, 2002).

First, the geometric-passive NLSF control problem is solved, with CL globally-robustly stable dynamics accompanied by a Lyapunov function in analytic form. Then, classic dynamics and nonlinear observer theory are applied to solve the nonlocal robust OF stabilization problem with nonlinear and linear PID control schemes, including: (i) solvability, (ii) systematic construction with reduced model dependency, and (iii) simple tuning.

2. CONTROL PROBLEM

Consider a (possibly OL unstable) single-reactant *exothermic continuous reactor*, where a reactant is converted into product via a first-order reaction rate ($c\alpha$) with Arrhenious temperature dependency (α), according to the dimensionless dynamic mass and heat balances (Aris, 1969)

$$\dot{c} = \theta c_e - \lambda_c(\tau,\theta)c, \qquad c(0) = c_o \qquad (1a)$$
$$\dot{\tau} = c\alpha(\tau) - \eta(\tau,\theta,\tau_e,\tau_c), \qquad \tau(0) = \tau_o \qquad (1b)$$
$$z = mc + \tau, \quad y = \tau. \qquad (1c)$$

where $\alpha(\tau) = \exp(a_\alpha - \varepsilon_a/\tau)$, $\lambda_c(\tau,\theta) = \theta + \alpha(\tau)$

$$\eta(\tau,\theta,\tau_e,\tau_c) = \lambda_\tau(\theta)\tau - (\theta\tau_e + \upsilon\tau_c), \ \lambda_\tau(\theta) = \theta + \upsilon$$

c (or τ) is the concentration (or temperature) *state*, υ is the heat transfer number, θ is the measured volumetric flow rate input, a_α is frequency factor-Damokholer number product, ε_a

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is the activation energy, y is the measured output temperature, τ_e (or c_e) is the measured (or unmeasured) feed temperature (or concentration), the coolant temperature τ_c is the *control input*, and z is the regulated output. In compact vector notation, reactor (1) is written as

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, w, \boldsymbol{d}, u), \quad \boldsymbol{x}(0) = \boldsymbol{x}_o, \quad y = \boldsymbol{c}_y \boldsymbol{x}, \quad z = \boldsymbol{c}_z \boldsymbol{x} \qquad (2)$$

where $\boldsymbol{x} = (c, \tau)^T$, $w = c_e$, $\boldsymbol{d} = (\theta, \tau_e)^T$
$u = \tau_c$, $\boldsymbol{c}_x = (0\ 1)^T$, $\boldsymbol{c}_z = (m\ 1)^T$

$\boldsymbol{x}$ is the *state*, $\boldsymbol{d}$ (or w) is the *measured* (or *unmeasured*) *input*, and y (or z) is the *measured* (or *regulated*) output, and the constant m (1c) is an *adjustable parameter* for control design. For nominal input $(\bar{w}, \bar{\boldsymbol{d}}, \bar{u})$, the reactor *statics*, with n_s SSs $\bar{\boldsymbol{x}}_i$, are

$$\boldsymbol{f}(\bar{\boldsymbol{x}}_i, \bar{w}, \bar{\boldsymbol{d}}, \bar{u}) = 0, \bar{y}_i = \boldsymbol{c}_x \bar{\boldsymbol{x}}_i, \bar{z}_i = \boldsymbol{c}_z \bar{\boldsymbol{x}}_i, i = 1, \ldots, n_s \geq 1$$

Depending on its parameters, the OL reactor (2) has simple or complex nonlinear dynamics (Uppal et al., 1974). To the mass-heat reactor balance (2) we will refer to as *Cartesian dynamics*.

The problem is to design a dynamic OF stabilizing controller

$$\dot{\boldsymbol{\xi}} = \boldsymbol{g}_\xi(\boldsymbol{\xi}, \boldsymbol{d}, y), \quad \boldsymbol{\xi}(0) = \boldsymbol{\xi}_o, \quad u = \mu_y(\boldsymbol{\xi}, \boldsymbol{d}, y) \qquad (3)$$

so that the CL reactor is robustly stable about its (possibly OL unstable) nominal SS $\bar{\boldsymbol{x}}$, with: (i) solvability conditions, and (ii) simple construction (with model dependency, nonlinearity and coupling as small as possible) and tuning. We are interested in identifying the trade-off between response speed, robustness and control effort, and rigorously connecting advanced nonlinear (passive and dissipative) and industrial (PID) control. AA's reactor (Aris, 1969) is chosen as case example, with a stable focus $\bar{\boldsymbol{x}}_f$ (or node $\bar{\boldsymbol{x}}_n$), and an unstable SS (saddle $\bar{\boldsymbol{x}}$):

$$\bar{\theta} = \bar{c}_e = \upsilon = 1, \quad \bar{\tau}_e = \bar{\tau}_c = 7/4, \quad a_\alpha = 25, \quad \varepsilon_a = 50 \qquad (4)$$

$$\bar{\boldsymbol{x}}_f \approx (0.089, 2.206)^T, \bar{\boldsymbol{x}} = (0.5, 2)^T, \bar{\boldsymbol{x}}_n \approx (0.964, 1.768)^T \qquad (5)$$

3. OPEN-LOOP DYNAMICS

Here the global NL OL reactor dynamics are characterized with notions and tools from nonlinear dynamics and classical mechanics.

3.1 Cartesian dynamics

The reactor SSs are in the line set L, which is inscribed in the trapezoidal invariant set X (Alvarez et al., 1991; Alvarez et al., 2015), i.e.,

$$\bar{\boldsymbol{x}}_{i=1,\ldots n_s} \in L = \{\boldsymbol{x} \in \Re^2 | 0 \leq x_1 \leq c_e,\ x_2 = \tau_L^+ - m_L x_1\} \quad (6a)$$

$$L \subset X = \{\boldsymbol{x} \in \Re^2 | 0 \leq x_1 \leq c_e,\ \tau_L^- \leq \tau \leq \tau^+(x_1)\} \subset \Re^2 \quad (6b)$$

where $m_L = 1/(1+\upsilon)$, $\tau_L^- = (\tau_e + \upsilon\tau_c)/(1+\upsilon)$,
$\tau_L^+ = \tau_L^- + m_L c_e$, $\tau^+(x_1) = \tau_L^+ + m_L(c_e - x_1)$

X is an *invariant* set in the sense that any state motion $\boldsymbol{x}(t)$ born in X stays in X (Hubbard and West, 1995).

The reactor example (4) has two invariant sets contained in X (6b) (see Fig. 1): (i) the separatrix curve S_r that contains the saddle $\bar{\boldsymbol{x}}$ and divides the bassins of attraction X_p^f and X_p^n of the stable focus $\bar{\boldsymbol{x}}_f$ and node $\bar{\boldsymbol{x}}_n$, respectively, and (ii) the curve S_a that connects the three SSs. The curve S_a (or S_r) is an attractive (or repulsive set) with respect to X. The geometry of the OL dynamics of the reactor example (4) is presented in Fig. 1, including: (i) the romboid (yellow) set where the invariants curves S_r (or S_a) are reasonably close to their tangent line sets L_s (or L_u) at the unstable saddle SS $\bar{\boldsymbol{x}}$, and (ii) the romboid (with slashed boundary) where the reactor is expected to operate. These observations suggest that the m-parametric lines about L_s as set of regulated outputs (1c).

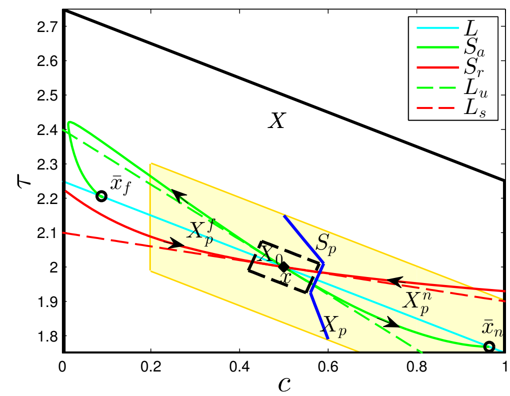

Fig. 1. Geometry of the OL Cartesian reactor dynamics.

Due to Bendixon-Poincare's theorem (Hubbard and West, 1995), each motion $\boldsymbol{x}(t)$ reaches asymptotically (with characteristic time t_x) either a SS point $\bar{\boldsymbol{x}}$ or a closed orbit $\bar{\boldsymbol{x}}(t)$ (Alvarez et al., 1991), i.e.,

$$\boldsymbol{x}_o \in X \Rightarrow \boldsymbol{x}(t) \in X, \quad \boldsymbol{x}(t) \xrightarrow{t_x} \bar{\boldsymbol{x}} \text{ or } \bar{\boldsymbol{x}}(t) \subset X. \qquad (7)$$

By virtue of Lyapunov's converse and La Salle's invariance theorems (La Salle and Lefschetz, 1960), there exists an "abstract" energy function $\varepsilon(\boldsymbol{x})$ with dissipation function $\boldsymbol{\Delta}(\boldsymbol{x})$:

$$e = \varepsilon(\boldsymbol{x}) \geq 0,\ \dot{e} = \boldsymbol{\Delta}(\boldsymbol{x}) \leq 0\ \forall\ \boldsymbol{x} \in X, \Delta(\boldsymbol{x}) = 0\ \forall\ \boldsymbol{x} \in \mathcal{N} \quad (8)$$

$$\Delta(\boldsymbol{x}) = d_{\boldsymbol{f}(\boldsymbol{x},\bar{w},\bar{\boldsymbol{d}},\bar{u})}\varepsilon(\boldsymbol{x}), \mathcal{N} = \{\boldsymbol{x} \in X | \Delta(\boldsymbol{x}) = 0\} \supseteq \mathcal{L}$$

where $d_{\boldsymbol{f}}\varepsilon$ is the directional derivative of ε along $\boldsymbol{f}$, and the union of limit sets $\mathcal{L}$ is the largest invariant set contained in the null dissipation set $\mathcal{N}$.

When reactor (2) (Alvarez et al., 2015) is *monostable* with global attractor $\bar{\boldsymbol{x}}$, $e = \varepsilon(\boldsymbol{x})$ is a single-well (Lyapunov) function with global minimum at $\bar{\boldsymbol{x}}$. When reactor (2) is *bistable*, as in example (5), $e = \varepsilon(\boldsymbol{x})$ is a two-well surface with local minima at $\bar{\boldsymbol{x}}_f$ and $\bar{\boldsymbol{x}}_n$, a saddle (in between) at $\bar{\boldsymbol{x}}$, and global minimum at the strongest attractor ($\bar{\boldsymbol{x}}_f$ or $\bar{\boldsymbol{x}}_n$). When reactor (2) has a *limit cycle* with unstable focus $\bar{\boldsymbol{x}}_f$ and orbit curve C_l, $e = \varepsilon(\boldsymbol{x})$ is a sombreroid surface with global minimum set (or maximum point) at C_l (or $\bar{\boldsymbol{x}}_f$).

3.2 Newtonian dynamics

Denote by

$$p = \tau, \quad v = \dot{\tau}, \quad a = \dot{v} = \ddot{\tau} \qquad (9)$$

the reactor temperature "position" p, "velocity" v and "acceleration" a, and apply the coordinate change

$$p = \tau := \sigma_p(\tau), \qquad v = \sigma_v(c, \tau, \boldsymbol{d}, u) \qquad (10a)$$