European Symposium on Computer Aided Process Engineering – 15
L. Puigjaner and A. Espuña (Editors)

A Systematic Approach to Plant-Wide Control Based On Thermodynamics

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Abstract

In this work, a systematic approach to plant-wide control design is proposed. The approach combines ingredients from process networks, thermodynamics and systems theory to derive robust decentralized controllers that will ensure complete plant stability. The proposed methodology will be illustrated on a reactor network exhibiting complex behaviour.

Keywords: Plant-wide Control, Process Networks, Irreversible Thermodynamics, Inventory Control.

1. Introduction

Over the years the area of plant-wide control has attracted the process engineering community as a challenging problem which drives continuing research efforts. A number of solutions to it were suggested, lying in between the following two extremes: a hierarchical decomposition of the original problem based on heuristic rules (Buckley, 1964; Luyben et al., 1997; Skogestad, 2002) and a mathematically oriented approach based on the solution of a given large scale mixed integer nonlinear programming dynamic optimization problem (see Biegler and Grossman, 2004, for an excellent review). Unfortunately, both lines of attack are hampered by a number of drawbacks which prevent their systematic application to general classes of process plants: the hierarchical approach usually leads to conflicting decisions only unravelled on a case by case basis and the mathematically one is limited by the high dimensionality of the problem and the restrictions imposed by the definition of the objective function. To overcome these issues, we combine previous results that link thermodynamics with passivity and Lyapunov theory (Farschman et al., 1998; Hangos et al., 1999; Alonso and Ydstie, 2001), and apply them to systematically design and/or to analyse stable decentralized control structures for process plants. In this way, the approach leads to hierarchical decentralized control structure which simultaneously ensures convergence of mass and energy inventories and guarantees robust stabilization of the intensive variables. The paper is structured as follows: In section 2, a formal representation of chemical process plants in terms of interconnected mass and energy networks is presented. The thermodynamic formalism and its consequences in designing decentralized controllers are presented in section 3. Finally, in Section 4 the approach is illustrated on a reaction network.

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2. The Underlying Structure of Process Networks

A process network is defined by a number *j=1,..., n* of well mixed homogeneous material regions connected by material and energy fluxes we will refer to as nodes, plus an extra region $j = 0$ which represents the environment. To each node *j* in the network we associate a state vector $z_j \in \mathbb{R}^{c+1}$ of the form $z_j=(n_1^j,...,n_c^j,u^j)^T$, where n_i^j represents the mole numbers of component *i*, u^j is the internal energy and *c* stands for the total number of chemical species. Nodes and environment are connected by a set of *n* convective fluxes we refer to as $f_j \in \mathbb{R}^{+c}$ and $p_j(f_j) \in \mathbb{R}^{+}$ for component and energy, respectively. Since energy is transported through material flows, we also have that $p_j(0) = 0$. Note that the formalism as it stands can easily accommodate multiple connections between modes by defining $\phi_j = \sum_{k=1}^{n} \alpha_{jk} \phi_j$, where ϕ_j stands for either material or energy fluxes and α_{jk} represents the fraction of ϕ_j directed to the node *k* so that $\sum_{k=1}^{n} \alpha_{jk} = 1$ (Hangos et al., 1999).Dissipative transfer between nodes in the network is included through vectors $\varphi^k \in \mathbb{R}^{+d_c}$ (with $i=1...,c$) and $\psi \in \mathbb{R}^{+d_u}$ which stand for mass and energy respectively. Network dynamics obey standard conservation principles for mole number and energy which, with some abuse of notation, can be formally stated as:

$$\dot{n}^k = N_\phi f^k + N_\varphi \varphi^k + \nu W \qquad n^k, f^k \in \mathbb{R}^{+n}; k = 1,\ldots,c; \tag{1}$$

$$\dot{u} = N_\phi p + N_\psi \psi + Q \qquad u, p \in \mathbb{R}^{+n} \tag{2}$$

where $N_\phi \in \mathbb{R}^{n \times n}$ denotes a convective column conservation matrix (Hangos et al., 1999). $N_\varphi \in \mathbb{R}^{n \times d_c}$, $N_\psi \in \mathbb{R}^{n \times d_u}$ are matrices which define network dissipative transfer interconnections, and the extra-terms *vW* and *Q* in Eqns (1)-(2) have been included to account for chemical reaction units and external heat sources, respectively. Alternative network dynamic representations can be derived from the fundamental network dynamics (1)-(2). In this way, the corresponding *mass network representation* can be easily obtained by defining transformations $m = \sum_{k=1}^{c} \sigma_k n^k$ and $\phi = \sum_{k=1}^{c} \sigma_k f^k$ with σ_k being molecular weight of the *k*-specie. *Inventory network representations* will result from projecting Eqns (1)-(2) onto the linear operators $P_\varphi \in \mathbb{R}^{n-d_c \times n}$ and $P_\psi \in \mathbb{R}^{n-d_u \times n}$ satisfying $P_\varphi \left[N_\varphi \nu \right] = 0$ and $P_\psi \left[N_\psi \nu \right] = 0$, respectively, so that:

$$\dot{n}_I^k = N_\phi f_I^k \qquad n_I^k, f_I^k \in \mathbb{R}^{+(n-d_c)}; k = 1,\ldots,c; \tag{3}$$

$$\dot{u}_I = N_\phi p_I \qquad u_I, p_I \in \mathbb{R}^{+(n-d_u)} \tag{4}$$

3. Hierarchical Design of Decentralized Controllers

3.1. Thermodynamic foundations of Process Networks

To start with, we consider that each node in the process network with volume ν_j is equipped with a continuous and twice differentiable scalar function $S_j\left(z_j, \nu_j\right): \mathbb{R}^{+(c+2)} \mapsto \mathbb{R}$ with the following properties:

1. $S_j\left(z_j, v_j\right)$ is a first order homogeneous function in all their arguments so that

$$S_j = \mu_j^T z_j + \mu_v v_j \tag{5}$$

2. $S_j\left(z_j, v_j^*\right)$ is strictly concave with respect to the vector z_j.

Function S_j, as defined, coincides with classical entropy (Callen, 1985). From Property 1, it follows that entropy is an additive function so that for a process network its total entropy is of the form $S = \sum_{j=1}^{n} S_j\left(z_j, v_j\right)$. Property 2 ensures that for (z,v) constants, S has a maximum over the convex set:

$$C = \left\{ (z_j, v_j)_{j=1}^n \;\middle|\; \sum_{j=1}^{n} z_j = z, \sum_{j=1}^{n} v_j = v \right\} \tag{6}$$

This, in fact, constitutes an evolution criterion as any thermodynamic system evolves in C so to maximize S. Finally, concavity also ensures the existence of a well defined one-to-one map between the vector of intensive properties μ_j and the vector of densities $\rho_j = v_j^{-1} z_j$. One main implication, of interest in process networks, is that whenever $\phi = 0$ network states will evolve so to maximize S. This can be easily shown by noting that $\phi = 0 \Rightarrow f^k = 0$ for $k = 1,...,c$ and $p(0) = 0$ so that Eqns (3)-(4) become $\dot{n}_I^k = \dot{u}_I = 0$. Since material and energy inventories are constant, we are in the set C and the evolution criterion applies. It is worth mentioning that as the network evolves, entropy is being produced so by computing the time derivative of S along (1)-(2) we obtain:

$$\dot{S} = P_s \quad with \quad P_s = \sum_i \sum_j \left[\varphi_{ij} \quad \psi_{ij} \right](\mu_i - \mu_j) \geq 0 \tag{7}$$

Since S is bounded from above by its maximum, we also have that $P_s\left(z_j^*\right) = 0$ for $\left(z_j^*\right)_{j=1}^n = Arg\ \underset{C}{Max}\ S$, the *equilibrium state* of the network. The entropy balance represented by Eqn (7) adopts the following form for open process networks:

$$\frac{dS}{dt} = P_s + \Phi_s(\mu_j, \phi) \tag{8}$$

where $\Phi_s\left(\mu_j, \phi\right)$ denotes the entropy flow through the network, which by definition becomes zero at the equilibrium state of the network, i.e. $\Phi_s\left(\mu_j^*, \phi\right) = 0$.

3.2. Decentralized control design

In order to preserve and/or to enforce the stability of extensive as well as intensive plant states, we make use of previous results in system theory that links thermodynamics with passivity and Lyapunov theory (Hangos et al, 1999; Alonso and Ydstie, 2001). The underlying idea is to exploit the concavity of the entropy function to construct natural storage and Lyapunov candidates and to employ them to design stabilizing (usually high gain) controllers. However, as discussed previously, concavity can only be attained once the network states are in the set C defined in (6). This fact, motivates a hierarchical control design decomposition in which mass and energy inventory controllers are first designed to ensure that the network states will remain in the set C. In particular, the

mass and energy inventory control layers consist of linear proportional controllers of the form:

$$\phi_I = \phi_I^* + \omega_m \left(m_I - m_I^* \right) \qquad p_I = p_I^* + \omega_u \left(u_I - u_I^* \right) \tag{9}$$

where ω_m and ω_u are appropriate gain matrices constructed so that $N_\phi \omega_m$ and $N_\phi \omega_u$ are negative definite. By applying (9) to the inventory network (3)-(4), it is straightforward to show that $m_I \to m_I^*$ and $u_I \to u_I^*$ exponentially fast. Integral action could be also included in (9) without substantially altering the stability properties of the closed loop network (Farschman et al, 1998). From the thermodynamic properties discussed in Section 3.1, it also follows that since the network states are in the interior of the set *C*, its entropy will remain upper and lower bounded and consequently, from Eqn (8), we have that:

$$\lim_{T \to \infty} \int_0^T (P_s + \Phi_s) d\tau = 0 \tag{10}$$

Unfortunately, condition (10) does not prevent the density states $\rho_j = \nu_j^{-1} z_j$, and thus their intensive counterparts from exhibiting complex dynamic behaviour such as multiplicities. However, since the network remains in *C*, the network entropy is strictly concave and intensive variable control can be designed by, for instance, methods discussed in Alonso and Ydstie (2001) to ensure convergence of the network density states. This will be illustrated next on a representative example.

4. Case Study: A Non-isothermal CSTR

We illustrate the proposed hierarchical control design methodology on a jacketed non-isothermal CSTR in which an liquid phase irreversible exothermic reaction $A \rightarrow B$ takes place. A detailed description of the process model and parameters can be found in Alonso and Banga (1998).

4.1. Mass and energy inventory control

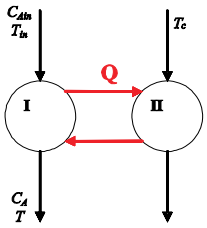
Figure 1 depicts a schematic representation of the reactor and heat exchanger as a process network consisting of two nodes connected by a dissipative heat transfer term. The mass and energy inventory control approach discussed in Section 3.2 is diagrammatically represented in Figure 2. As shown in the Figure, mass inventory control results into a LC control loop which fix the residence time in the reactor. In order to implement the energy inventory control, an internal energy observer was designed to estimate the energy content in the reactor, and the estimate used as the measurement for the FC loop acting on coolant flow rate. As discussed previously, the proposed controllers guarantee inventories to converge to the desired set-point. However, the control structure does not ensure control of temperature and conversion in the reactor. Such behaviour motivates the thermodynamic analysis presented next.

4.2. Thermodynamic analysis of the reactor network.

The inventory control structure allows us to re-write process network dynamics in terms of intensive variables, which for this case takes the form:

$$\dot{C}_A = -\rho + \theta \left(C_A^{in} - C_A \right) \qquad \dot{T} = \beta \rho + \theta \left(T_{in} - T \right) - \gamma \left(T - T_c \right) \tag{11}$$

where C_A and T are composition and temperature, respectively. ρ is the reaction rate and θ, β, and γ are dimensionless physical parameters related with residence time and heat transfer areas (see Alonso and Banga, 1998).



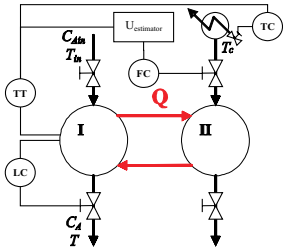


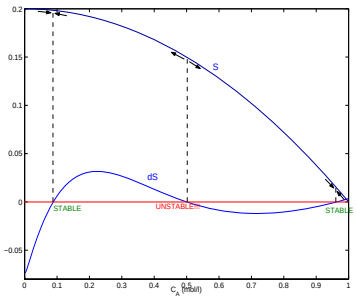
Figure 1. Reactor process network *Figure 2. Proposed control structure*

The entropy balance associated to this network takes the form given in (8) with entropy production and entropy flow being of the form:

$$P_s = \gamma\left(\frac{1}{T_c}-\frac{1}{T}\right)(T-T_c)-\frac{R}{dc_p}\rho\frac{\mu_B-\mu_A}{T} \tag{12}$$

$$\phi_s = \frac{1}{T}\left[\frac{C_A^{in}c_{p_A}(T_{in}-T)}{dc_p}+\beta\left(C_A-C_A^{in}\right)\right]\theta-\frac{\Delta\mu}{Tdc_p}\left(C_A^{in}-C_A\right)\theta-\frac{\gamma}{T_c}(T-T_c) \tag{13}$$

Process entropy and its time derivative (which equals $P_s+\Phi_s$) is represented in Figure 3 along the set C defined by (6), which in our case corresponds with the manifold of constant mole number and energy. As it can be seen from the Figure, there are three points in C satisfying the steady-state entropy balance which correspond with an unstable and two stable stationary points. Note that the stability or instability can be easily established from the curvature of the systems entropy.



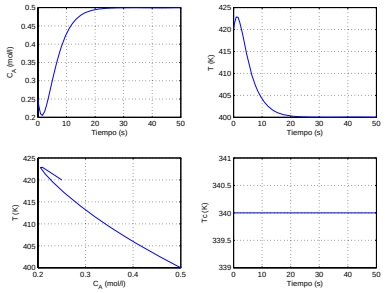


Figure 3. Steady states stability analysis using S *Figure 4. Concentration and Temperature evolution under intensive variable control*

4.3. Intensive variables control

In order to ensure stabilization of the intensive variables (reactor concentration and temperature) the inventory control configuration is completed with an intensive variable control loop acting on the coolant temperature T_c. Although different control structures could serve to that purpose, in this work a PI temperature controller and a non-linear exact linearizing control (Alonso and Banga, 1998) were tested, demonstrating for both

cases state stabilization. The evolution of temperature and concentration under intensive variable control is presented in Figure 4. Finally, some control experiments were carried out in order to test the unstabilizing effect of input constraints on the closed loop dynamics. In this case, the thermodynamic analysis reveals new points in the region *C* satisfying the stationary entropy balance (see Figure 5) which corresponds with either stable, unstable or even limit cycles caused by total inventory fluctuations. A representation of one of such oscillatory regimes is depicted in Figure 6.

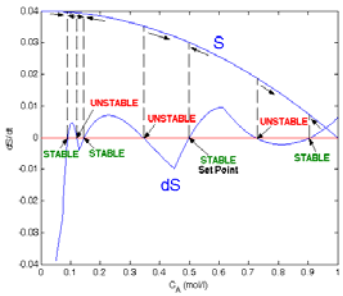


Figure 5. Stability analysis using entropy

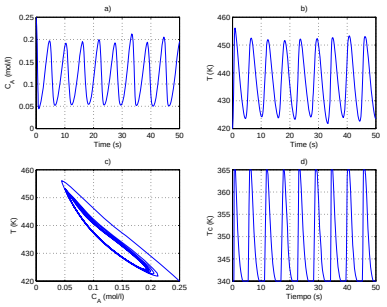


Figure 6.Evolution of the state and manipulated variable in the presence of input constraints

5. Conclusions

In this contribution, a systematic plant-wide control design methodology has been presented. The approach, which combines tools and concepts from systems theory and thermodynamics, allows the design of decentralized control structures which ensure stabilization of both plant extensive and intensive variables. The proposed methodology has been illustrated on a reactor network exhibiting complex behaviour.

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Acknowledgements

The authors acknowledge the financial support received from the Spanish Government (MCyT Projects PPQ2001-3643) and Xunta de Galicia (PGIDIT02-PXIC40209PN).