Dissipative boundary PI controller for an adiabatic plug-flow reactor with mass recycle

M.A. Zárate-Navarro[1] J.P. García-Sandoval[1] S. Dubljevic[2]

[1]Departamento de Ingeniería Química
Universidad de Guadalajara, México (paulo.garcia@cucei.udg.mx)

[2]Chemical & Materials Engineering Department
University of Alberta, Canada (Stevan.Dubljevic@ualberta.ca)

3rd IFAC Workshop on Thermodynamic Foundations for a Mathematical Systems Theory

Outline

1. Motivation
   - Introduction
   - Convective Distributed Parameter System with mass recycle
2. Dissipative properties and boundary control
   - Dissipative properties
   - Boundary control
3. Case study
   - Mass and energy balances
   - Numerical simulations

Outline

Introduction

- Dissipation, storage function and supply rate (Willems, 1972).
- Stability analysis based on the internal entropy production (García-Sandoval et al., 2016).
- Tubular reactors with mass recycle (Reilly and Schmitz, 1966).
- Using thermodynamic properties to regulate nonlinear systems such as plug flow reactors is still an open field.

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System description

- Convective Distributed Parameter System

$$\frac{\partial \eta(z,t)}{\partial t} = -v\frac{\partial \eta(z,t)}{\partial z} + Mf(\zeta), \qquad (1)$$

where: state vector $\eta(z,t) \in \mathcal{H}^n[(0,L),\mathbb{R}^n]$ (extensive properties) and are the respective entropy-conjugated co-states $\zeta(z,t) \in \mathcal{H}^n[(0,L),\mathbb{R}^n]$ (intensive properties). $z \in [0,L] \subset \mathbb{R}$, $t \in [0,\infty]$, $v = \frac{F}{A} \in \mathbb{R}^+$.

- Initial conditions:

$$\eta(z,0) = \alpha(z), \qquad (2)$$

where $\alpha(z) \in \mathcal{H}^n[(0,L),\mathbb{R}^n]$.

- Boundary condition with mass recycle:

$$\eta(0,t) = (1-u(t))\,\eta_{in}(t) + u(t)\,\eta(L,t). \qquad (3)$$

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Entropy balance

- Entropy as a state variable: $s = \phi(\eta)$.
- Entropy gradient:

$$\zeta(z,t) := \nabla s(z,t), \tag{4}$$

- Given the Gibbs relation: $ds = \zeta^{\mathsf{T}} d\eta$, the entropy dynamics is:

$$\frac{\partial s(z,t)}{\partial t} = -v \frac{\partial s(z,t)}{\partial z} + \sigma(z,t), \tag{5}$$

where $\sigma(z,t) := \zeta^{\mathsf{T}} Mf(\zeta)$ is the internal entropy production density.
- Total entropy: $S(t) = A\int_0^L s(\lambda,t)\,d\lambda$, with dynamics

$$\frac{dS(t)}{dt} = -F\left[s(L,t) - s(0,t)\right] + \Sigma(t), \tag{6}$$

where $\Sigma(t) = A\int_0^L \sigma(\lambda,t)\,d\lambda \geq 0$.

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Outline

Entropy as storage function

Proposition

Consider a convective thermodynamic system as the previously described with constant velocities (Eqs. (1)-(3)*). If the system is thermodynamically consistent, then it is dissipative with the entropy as the storage function and the internal entropy production as the dissipation.*

Proof.

(Sketch) Let us consider $W(t) := \bar{S} - S(t)$, then $\frac{dW(t)}{dt} = F\left[s(L,t) - s(0,t)\right] - \Sigma(t)$. Since $\Sigma(t) \geq 0$, $W(t) - W(0) \leq \int_0^t \omega\left(\eta_0(\theta), \eta_L(\theta)\right) d\theta$, with $\omega\left(\eta_0(t), \eta_L(t)\right) := F\left[s_L(t) - s_0(t)\right] = F\left[s(L,t) - s(0,t)\right]$. □

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Outline

Boundary control definition

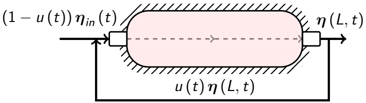

Figure: System with mass recycle.

- Disturbance vector: $\mathbf{d}(t) := \boldsymbol{\eta}_{in}(t)$,
- Regulated variable: $y(t) := \eta_i(L, t)$,
- Control variable: $u(t)$ (recycle rate).

- Boundary condition: $\boldsymbol{\eta}(0, t) = (1 - u(t))\,\mathbf{d}(t) + u(t)\,\boldsymbol{\eta}(L, t)$.

Controller structure

General controller

A controller that solve the problem is:

$\dot{u}(t) = (\dot{\chi}_{ref}(t) - \kappa_1 e_1 - w(t))/\Phi(t)$,

where $e_1(t) = \chi(t) - \chi_{ref}(t)$, $\Phi(t) := F\zeta_0^T(t)[\boldsymbol{\eta}_L(t) - \mathbf{d}(t)]$, $\zeta_0(t) = \zeta(0,t)$ and $\boldsymbol{\eta}_L(t) = \boldsymbol{\eta}(0,t)$, while $\dot{\chi}_{ref}(t)$ is the reference of $\chi(t) := dW/dt$ (storage function dynamics). Finally, $w(t) := \frac{d^2W}{dt^2} + F\zeta_0^T(t)[\boldsymbol{\eta}_L(t) - \mathbf{d}(t)]\dot{u}(t)$.

Particular controller

Considering a PI structure for $\dot{\chi}_{ref}(t)$ the controller reduce to

$\dot{u}(t) = \left(K_p e_2(t) + \frac{K_p}{\tau_I}\int_0^t e_2(\tau)\,d\tau\right)/\Phi(t)$,

where, $e_2 = y(t) - y_{ref}$, while K_p and τ_I are the tuning parameters.

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Model: Single reversible reaction: $E_1 \rightleftharpoons 2E_2$

- Mass and internal energy balances:

$$\begin{aligned}\frac{\partial C_i(z,t)}{\partial t} &= -v\frac{\partial C_i}{\partial z} + \Gamma_i r, \quad i = 1,2\\ \frac{\partial U(z,t)}{\partial t} &= -v\frac{\partial U}{\partial z}\end{aligned}$$

where $\mathbf{C}^{\mathrm{T}}(z,t) = (C_1\ C_2)$, $U(z,t) = \mathbf{C}^{\mathrm{T}}\mathbf{u}$,
$\mathbf{u} = \mathbf{u}_{ref} + \int_{T_{ref}}^{T} \mathbf{c}_v dT$, $r(z,t) = k\left(X_1 - K_{eq}X_2^2\right)$ with
$k = D_R \exp\left(-\frac{\varepsilon_0\left(\Gamma^{\mathrm{T}}\boldsymbol{\mu}^{\circ}\right)+E_{a0}}{RT}\right)$ and $K_{eq} = \exp\left(\frac{\Gamma^{\mathrm{T}}\boldsymbol{\mu}^{\circ}}{RT}\right)$.

- Boundary conditions of the system are

$$\mathbf{C}(0,t) = (1-u(t))\,\mathbf{d}_1(t) + u(t)\,\mathbf{C}(L,t), \tag{7}$$

$$U(0,t) = (1-u(t))\,d_2(t) + u(t)\,U(L,t). \tag{8}$$

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Parameters and space-time variation

Parameter	Value
R (J/mol·K)	8.314
$\mathbf{s}_{ref}^{T}/R$ (-)	(30.06 10.82)
$\mathbf{u}_{ref}^{T}/R$ (K)	$(1.623\ 0.481)\times10^4$
$\mathbf{c}_{p}^{T}/R$ (-)	(21.65 10.22)
ε_0 (-)	0.5
E_{a0}(J/mol)	2.2×10^5
D_R(1/h)	1.0×10^{20}
K_p/F(h/m^3)	1.5×10^4
$1/\tau_I F$(1/m^3)	0.18

Table: Thermodynamic properties and parameters for the numerical

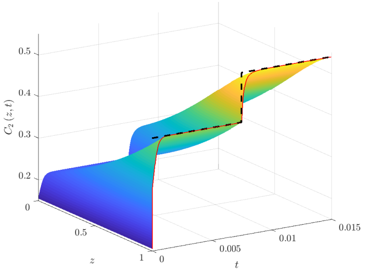

Figure: $C_{2,L}(t)$ regulation with a set point change at $t = t_{end}/2$.

$\Phi(t)$, supply rate and manipulate variable

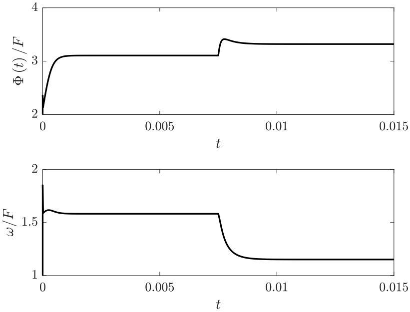

Figure: $\Phi(t)$ function and supply rate per flow.

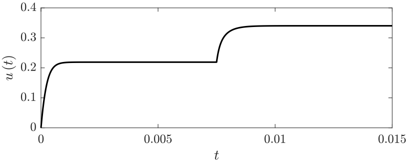

Figure: Manipulated variable.

Space-time variation, entropy and internal entropy production

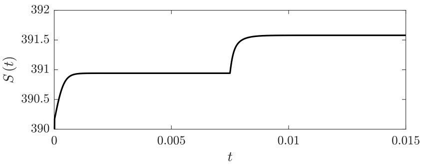

Figure: Entropy function.

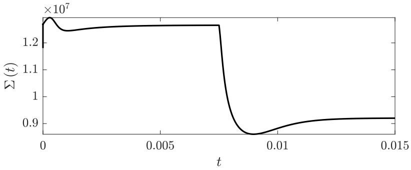

Figure: Internal entropy production.

Summary

- The proposed PI structure smoothly tracks a desired set point without offset.
- This structure is robust against uncertain terms, such as $\dot{\Sigma}$.
- Although the entropy function gives insight on dissipativity, it cannot give information on the stability of the desired set point.
- The internal entropy production gives the principles for further applications, such as optimization and its time derivative can determine the stability of a desired trajectory.

- Outlook
  - To define saturation constraints in order to overcome potential sign changes in the $\Phi(t)$ function.
  - Observer design to estimate unmeasured states.

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For Further Reading I

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Reilly, M., Schmitz, R., 1966. Dynamics of a tubular reactor with recycle: Part I. stability of the steady state. AIChE Journal 12 (1), 153–161.

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