Availability based Stabilization of Tubular Chemical Reactors

W. Zhou, F. Couenne, B. Hamroun, and Y. Le Gorrec*

LAGEP, UMR CNRS 5007- Université Lyon 1-France
* FEMTO-ST/AS2M, Besançon, France

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### Bibliography on the control of tubular reactors

- **Georgakis, et al. CES 1977**
- **LQ control**
  - Moghadama et al. Automatica 2013
  - Aksikas et al. Automatica 2009
- **Nonlinear control**
  - Hudon et al. CACE 2008 (Lyapunov based control)
  - Vilas et al. CES 2007 (robust NL control)
  - Cougnon et al. AICHE J 2006 (Lyapunov based control)
  - Bošković and Krstić CACE 2002 (backstepping control)
  - Christofides NA 2001 (Galerkin reduction and Lyapunov techniques)
- **Passive control design**
  - Ruszkowski et al. AIChE j 2005
  - Alonso and Ydstie Automatica 2001
Objectives

- Stabilization of a tubular reactor at the desired steady state profile \((z_d)\) using the thermodynamic availability \(A\) as Lyapunov function in the setting of the irreversible thermodynamics
- The distributed control variable \(T_j\)

Existing results

- Stabilization of non isothermal Continuous Stirred Tank Reactors (CSTR) (JPC, 2012, Hoang et al.)
The thermodynamic variables and main laws

- The extensive variables $z$
- The intensive variables $w$

- First law: conservation of the internal energy
- Second law: concavity of the entropy function w.r.t. element of $z$ (other than $s$) or $u$

The Gibbs equation and the Gibbs-Duhem equation

$$du = w^T dz \text{ and } u = w^T z \implies dw^T z = 0$$
The local equilibrium assumption for PDEs models

- Local state and specific properties are equivalent on small enough scales
- The Gibbs equation becomes \((\nu\) is the mean velocity\)

\[
\frac{Du}{Dt} = w^T \frac{Dz}{Dt} \quad \text{with} \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \nu \frac{\partial}{\partial x}
\]

This formula is used to compute the irreversible entropy production \(\implies \partial_t s\)

The integral formulation in a simple 1D case

\[
\frac{d}{dt} \left( \int_{x_a+vt}^{x_b+vt} \rho u \right) = \left( \int_{x_a+vt}^{x_b+vt} \rho \frac{\partial u}{\partial t} \right) + [\nu \rho u]_{x_a+vt}^{x_b+vt} \\
= \int_{x_a+vt}^{x_b+vt} \left( \rho \frac{\partial u}{\partial t} + \nu \rho \frac{\partial u}{\partial x} \right)
\]
From this point: \( ds = w^t dz, \quad z^T = (u \ldots \omega_i) \) and \( w^T = \left( \frac{1}{T} \ldots \frac{-\mu_i}{T} \right) \)

The specific availability \( a = -(w - w_d)^T z \) is convex \( (s = w^T z) \) w.r.t. \( z \) and positive.
The availability function for PDEs models

The availability over a fixed domain A

\[ A(t) = \int_0^L a(x, t) = \int_0^L -(w(z) - w_d(x))^T z(x, t) \]

\[ \frac{dA(t)}{dt} = \frac{d}{dt} \int_0^L -(w - w_d)^T z \quad w^T z = s \]

\[ \frac{dA(t)}{dt} = \int_0^L \partial_t a = \]
\[ \int_0^L -(w(z) - w_d(x))^T \partial_t z + \nu \int_0^L \left( \frac{\partial (w(z) - w_d(x))}{\partial t} \right)^T z \text{ or} \]
\[ \frac{dA(t)}{dt} = \int_0^L \left( \partial_t s(x, t) - w_d^T \partial_t z(x, t) \right) \]
The main assumptions

- Only longitudinal axis is under consideration.
- The reacting mixture is ideal and incompressible.
- The pressure $P$ is constant.
- The average fluid velocity $v$ is constant.
- The linear density $\rho$ is constant.
- The chemical reaction $\nu_A A \rightarrow \nu_B B$. The kinetics $r$ is first order w.r.t. $A$. The kinetic constant is given by the Arrhenius law.
- The distributed heat exchange $q(x)$ with the jacket is given by $q(x) = C(T(x) - T_j(x))$ where $T_j(x)$ is the jacket temperature at $x$ and $T(x)$ the temperature in the reactor.
\[ \partial_t z = -\partial_x F + R + gq \]

with \( z = (\rho h \rho \omega_A \rho \omega_B) \), \( F = F_{\text{dis}} + F_{\text{conv}} \), \( R = (0 \ -r \ r)^T \) and \( g = (1 \ 0 \ 0)^T \).

**Boundary conditions**

- Continuity of flux at \( x = 0 \) (species, enthalpy)
- \( \partial z_x(t) \big|_L = 0 \)
Open loop simulation

\[
T_{\text{inlet}} = 330K, \quad w_{A_{\text{in}}} = 1 \quad \text{(initial state profile: } T_j(x, 0) = 350K) \\
T_{j_d}(x, 0) = 370K
\]

*Figure:* local availability function at L/120, L/2 and L
The control problem

The stabilization problem around a desired profile

The objective is that the closed loop dynamics of $A$ be s.t.

$$\frac{dA}{dt} \leq - \int_0^L (w - w_d)^T K (w - w_d)$$

Set $\tilde{w} = w - w_d$

$$\frac{dA(t)}{dt} = \int_0^L \partial_t a = \int_0^L -\tilde{w}^T \partial_t z + v \int_0^L \left( \partial_x \tilde{w} \right)^T z$$

Remind the dynamics: $\partial_t z = -\partial_x \mathbf{F} + R + gq$

$$\frac{dA(t)}{dt} = \left[ \tilde{w}^T \mathbf{F} \right]_0^L - \int_0^L \tilde{w}^T (R + gq(T_j)) - \int_0^L \left( \frac{\partial \tilde{w}}{\partial x} \right)^T \mathbf{F}_{\text{dis}} + \int_0^L \left( \frac{\partial w_d}{\partial x} \right)^T \mathbf{F}_{\text{con}}$$
The proposed solution

$T_j(x, t)$ as control variable only

$$
\frac{dA(t)}{dt} = \int_0^L \partial_t a = \int_0^L \tilde{w}^T \left( - \partial_x F + R + gq \right) + v \int_0^L \left( \partial_x \tilde{w} \right)^T z
$$

$$
q(x, t) = \frac{\tilde{w}^T \left( R + \partial_x F \right) + v \frac{\partial \tilde{w}}{\partial x}^T z + K \tilde{w}^T \tilde{w}}{\tilde{w}_h}
$$

It can be then easily deduced the distributed control

$$
T_j(x, t) = \frac{\tilde{w}^T \left( R + \partial_x F \right) + v \frac{\partial \tilde{w}}{\partial x}^T z + K \tilde{w}^T \tilde{w}}{C \tilde{w}_h} + T(x)
$$
The first simulation results

**Figure:** Profile at s=40s of temperature and the desired one (left with $T(x, 0) = T_d(x) - 10$ and right with $T(x, 0) = T_d(x) + 10$ in closed loop and open loop
Conclusion

- Improve the results
- Do the same procedure with the reduced availability $a_r$

$$a = \left( \frac{1}{T} - \frac{1}{T_d} \right) h + \left( -\frac{\mu_A}{T} + \frac{\mu_{A_d}}{T_d} \right) \rho \omega_A + \left( -\frac{\mu_B}{T} + \frac{\mu_{A_d}}{T_d} \right) \rho \omega_B \quad (1)$$

The chem. potential of species $i$ in an ideal mixture ($P = P_{ref}$):

$$\mu_i = \mu_{i_{ref}} + c_{p_i} (T - T_{ref}) - c_{p_i} T \ln\left( \frac{T}{T_{ref}} \right) + \overbrace{RT \ln(\omega_i)}^{\text{The mixing part}} + w_{ri}$$

The reduced availability:

$$a_r = \tilde{w}_h h + \tilde{w}_{r_A} \rho \omega_A + \tilde{w}_{r_B} \rho \omega_B$$

**Property**

$a_r$ is a positive quantity.
$T_{inlet} = 330K, w_{Ain} = 1$ (initial state profile: $T_j(x, 0) = 350K$)  
$T_{j_0}(x, 0) = 370K$

**Figure:** left: local reduced availability function at $L/120$, $L/2$ and $L$  
right: local a
Thank you for your attention ...