Availability based Stabilization of Tubular Chemical Reactors

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TFMST 2013 - 16 July 2013

Bibliography on the control of tubular reactors

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- LQ control
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  - Aksikas et al. Automatica 2009
- Nonlinear control
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  - 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

- 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 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

$du = w^T dz$ and $u = w^T z \Longrightarrow dw^T \, z = 0$

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

$\frac{Du}{Dt} = w^T \frac{Dz}{Dt}$ with $\frac{D}{Dt} = \frac{\partial}{\partial} + v\frac{\partial}{\partial}$ the material derivative

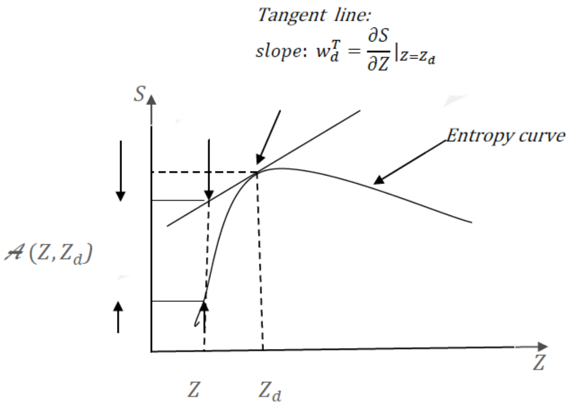
This formula is used to compute the irreversible entropy production $\Longrightarrow \partial_t s$

The integral formulation in a simple 1D case

$$\frac{d}{dt}\Big(\int_{x_a+vt}^{x_b+vt} \rho u\Big) = \Big(\int_{x_a+vt}^{x_b+vt} \rho\frac{\partial u}{\partial t}\Big) + [v\rho u]_{x_a+vt}^{x_b+vt}$$
$$= \int_{x_a+vt}^{x_b+vt} \Big(\rho\frac{\partial u}{\partial t} + v\rho\frac{\partial u}{\partial x}\Big)$$

From this point : $ds = w^t dz$, $z^T = \left(u \dots \omega_i\right)$ and $w^T = \left(\frac{1}{T} \dots \frac{-\mu_i}{T}\right)$

The specific availability $a = -(w - w_d)^T z$ is convex ($s = w^T z$) w.r.t. z and positive



The availability over a fixed domain A

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

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

$$\frac{dA(t)}{dt} = \int_0^L \partial_t a =$$

$$\int_0^L -(w(z) - w_d(x))^T \partial_t z + v \int_0^L \left(\frac{\partial(w(z) - w_d(x))}{\partial t}\right)^T z \text{ or}$$

$$\frac{dA(t)}{dt} = \int_0^L -\left(\partial_t s(x,t) - w_d^T \partial_t z(x,t)\right)$$

- 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 ρ is constant.
- The chemical reaction $\nu_A A \longrightarrow \nu_B B$. 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 $z = (\rho h \; \rho\omega_A \; \rho\omega_B)$, $F = F_{dis} + F_{conv}$,$R = \begin{pmatrix} 0 & -r & r \end{pmatrix}^T$ and $g = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix}^T$.

Boundary conditions

- Continuity of flux at $x = 0$ (species, enthalpy)
- $\partial z_x(t)|_L = 0$

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

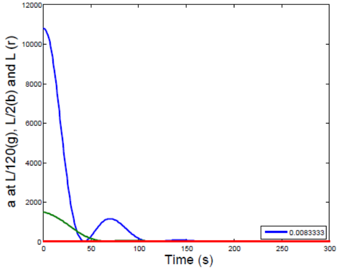


Figure: local availability function at L/120, L/2 and L

The 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: $\partial_t z = -\partial_x F + R + gq$

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

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

$$\frac{dA(t)}{dt} = \int_0^L \partial_t a = \int_0^L -\tilde{w}^T\Big(- \partial_x F + R + g{\color{red}q}\Big) + v\int_0^L \Big(\partial_x \tilde{w}\Big)^T z$$

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

It can be then easily deduced the distributed control

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

The first simulation results

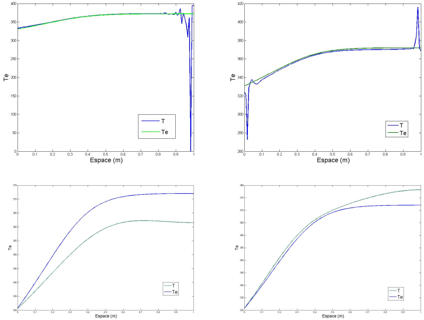


Figure: Profile at s=40s of temperature and the desired one (left with $T(x,0) = T_d(x) - 10$ and right with $T(x,0) = T_d(x) + 10$ in closed loop and open loop

Conclusion

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

$$a = (\frac{1}{T} - \frac{1}{T_d})h + (-\frac{\mu_A}{T} + \frac{\mu_{A_d}}{T_d})\rho\varpi_A + (-\frac{\mu_B}{T} + \frac{\mu_{A_d}}{T_d})\rho\varpi_B \quad (1)$$

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

$$\mu_i = \underbrace{\mu_{i_{ref}} + c_{p_i}(T - T_{ref}) - c_{p_i} T \ln(\frac{T}{T_{ref}})}_{w_{ri}} + \underbrace{RTln(\varpi_i)}_{The\ mixing\ part} .$$

The reduced availability :

$$a_r = \tilde{w}_h h + \tilde{w}_{r_A}\rho\varpi_A + \tilde{w}_{r_B}\rho\varpi_B$$

Property

a_r is a positive quantity.

$T_{inlet} = 330K, w_{A_{in}} = 1$ (initial state profile : $T_j(x,0) = 350K$)
$Tj_d(x,0) = 370K$

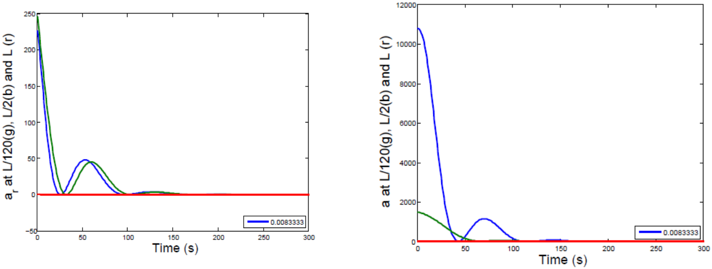


Figure: left: local reduced availability function at L/120, L/2 and L right: local a

Thank you for your attention ...