Passivity Based Control of Irreversible Port Hamiltonian Systems
Thermodynamic Foundations of Mathematical Systems Theory 2013

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Motivation and previous work

Motivation

Express the **first and second** principle of thermodynamics as a structural property of a quasi-port Hamiltonian system and use the structure for process control.

Previous work

- Many efforts to express simultaneously the conservation of energy and production of entropy (GENERIC, quasi Hamiltonian systems, Brayton-Mooser formulation,..)
  

- Use of thermodynamics in the design of passivity based controller
  
  [Alonso and Ydstie, 1996, Alonso and Ydstie, 2001, Hoang et al., 2011, Hoang et al., 2012]
Irreversible port Hamiltonian systems

H. Ramirez, B. Maschke and D. Sbarbaro, CES 2013, EJC 2013

A non-linear extension of port Hamiltonian systems
Port Hamiltonian systems

PHS are suited for modelling and control of (electro) - mechanical systems
[Maschke and van der Schaft, 1992, van der Schaft, 2000]

\[ \dot{x} = J(x) \frac{\partial U}{\partial x}(x) + g(x)u(t), \quad y = g(x)^\top \frac{\partial U}{\partial x}(x). \]

\( x \in \mathbb{R}^n, \ U : \mathbb{R}^n \to \mathbb{R} \) the Hamiltonian function, \( J(x) \in \mathbb{R}^n \times \mathbb{R}^n \) skew-symmetric structure matrix, \( g(x) \in \mathbb{R}^m \times \mathbb{R}^n \) the input map and \( u(t) \in \mathbb{R}^m \) is a time dependent input.

**Balance equations expressed by PHS**

- Conservation of the Hamiltonian and of Casimir’s of the Poisson bracket

\[ \frac{dU}{dt} = \frac{\partial U}{\partial x}^\top gu = u^\top y, \quad \frac{dC}{dt} = \frac{\partial C}{\partial x}^\top gu = u^\top y \]

- The Poisson bracket:

\[ \{Z, G\}_J = \frac{\partial Z}{\partial x}^\top (x)J(x)\frac{\partial G}{\partial x}(x). \]
Conservation of energy and irreversible entropy production

Many efforts to express the conservation of energy and production of entropy (GENERIC, quasi Hamiltonian systems, Brayton-Mooser formulation,...)

Simultaneous conservation of energy and irreversible entropy production

Consider a closed system:
\[
\frac{dU}{dt} = 0 \quad \text{and} \quad \frac{dS}{dt} = \sigma \left( x, \frac{\partial U}{\partial x} \right) \geq 0
\]

The second principle of thermodynamic requires \( J \) to explicitly depend on \( \frac{\partial U}{\partial x} \)

\[
\frac{\partial S}{\partial x}^\top J \left( x, \frac{\partial U}{\partial x} \right) \frac{\partial U}{\partial x} = \sigma \geq 0, \quad \text{for any } U(x)
\]

This is the reason to consider quasi Hamiltonian system

Retain much of the PHS structure, but their structure matrices depend explicitly on the gradient of the Hamiltonian.
Irreversible port Hamiltonian systems

We suggest a structure for quasi Hamiltonian systems: Irreversible port Hamiltonian systems

**IPHS for closed system**

\[
\dot{x} = R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)J \frac{\partial U}{\partial x}(x)
\]

i. \(x \in \mathbb{R}^n\), and \(U(x)\) and \(S(x)\) relates to the energy and entropy respectively.

ii. The constant structure matrix \(J = -J^\top \in \mathbb{R}^n \times \mathbb{R}^n\).

**The definition of \(R\)**

\[
R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right) = \gamma \left(x, \frac{\partial U}{\partial x}\right) \{S, U\}_J, \quad \gamma \geq 0.
\]

- \(\{S, U\}_J\) defines the thermodynamic driving force
- Entropy balance:

\[
\frac{\partial S}{\partial t} = \frac{\partial S}{\partial x}^\top RJ \frac{\partial U}{\partial x} = R\{S, U\}_J = \gamma \left(x, \frac{\partial U}{\partial x}\right) \{S, U\}_J^2 = \sigma \geq 0.
\]
Irreversible port Hamiltonian systems

**IPHS for open systems**

\[
\dot{x} = R \left( x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x} \right) J \frac{\partial U}{\partial x}(x) + W \left( x, \frac{\partial U}{\partial x} \right) + \sum_{i=1}^{m} g_i \left( x, \frac{\partial U}{\partial x} \right) u_i,
\]

i. \( x \in \mathbb{R}^n \), and \( U(x), S(x) : \mathbb{R}^n \rightarrow \mathbb{R} \) relates to the energy and entropy respectively.

ii. The constant structure matrix \( J = -J^\top \in \mathbb{R}^n \times \mathbb{R}^n \).

iii. \( W \in \mathbb{R}^n \) and \( g \in \mathbb{R}^n \) describes the interaction with the environment.

with

\[
R \left( x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x} \right) = \gamma \left( x, \frac{\partial U}{\partial x} \right) \{S, U\}_J, \quad \gamma \geq 0.
\]

**Energy balance and entropy balance with irreversible entropy creation.**

\[
\frac{dU}{dt} = \frac{\partial U}{\partial x}^\top \left( W + \sum_{i=1}^{m} g_i u_i \right), \quad \frac{dS}{dt} = \sigma + \frac{\partial U}{\partial x}^\top \left( W + \sum_{i=1}^{m} g_i u_i \right)
\]
The heat exchanger: interaction through two conducting walls

Consider two simple thermodynamic systems with entropy balance equations

$$\begin{bmatrix} \dot{S}_1 \\ \dot{S}_2 \end{bmatrix} = \lambda \begin{bmatrix} \frac{T_2(S_2) - T_1(S_1)}{T_1(S_1) - T_2(S_2)} \\ \frac{T_1(S_1) - T_2(S_2)}{T_1(S_1) - T_2(S_2)} \end{bmatrix} + \lambda_e \begin{bmatrix} 0 \\ \frac{u(t) - T_2(S_2)}{T_2(S_2)} \end{bmatrix}$$

with $x = [S_1, S_2]^T$ the entropies, $U = U_1(x_1) + U_2(x_2)$ the internal energy, $\frac{\partial U}{\partial x_i} = T_i(x_i) = T_0 \exp\left(\frac{x_i}{c_i}\right)$ where $T_0$ and $c_i$ are constants, $u(t)$ external heat source and $\lambda, \lambda_e > 0$ Fourier’s heat conduction coefficients of the wall.
The heat exchanger: interaction through two conducting walls

Consider two simple thermodynamic systems with entropy balance equations

\[
\begin{bmatrix}
\dot{S}_1 \\
\dot{S}_2
\end{bmatrix} = \lambda \begin{bmatrix}
\frac{T_2(S_2) - T_1(S_1)}{T_1(S_1) - T_2(S_2)} \\
\frac{T_1(S_1) - T_2(S_2)}{T_2(S_2)}
\end{bmatrix} + \lambda e \begin{bmatrix}
0 \\
\frac{u(t) - T_2(S_2)}{T_2(S_2)}
\end{bmatrix}
\]

with \( x = [S_1, S_2]^\top \) the entropies, \( U = U_1(x_1) + U_2(x_2) \) the internal energy, \( \frac{\partial U}{\partial x_i} = T_i(x_i) = T_0 \exp\left(\frac{x_i}{c_i}\right) \) where \( T_0 \) and \( c_i \) are constants, \( u(t) \) external heat source and \( \lambda, \lambda e > 0 \) Fourier’s heat conduction coefficients of the wall.

The process may be written as IPHS

\[
\begin{bmatrix}
\dot{x}_1 \\
\dot{x}_2
\end{bmatrix} = \lambda \left( \frac{1}{\partial U/\partial x_2} - \frac{1}{\partial U/\partial x_1} \right) \begin{bmatrix}
0 & -1 \\
1 & 0
\end{bmatrix} \begin{bmatrix}
\frac{\partial U}{\partial x_1} \\
\frac{\partial U}{\partial x_2}
\end{bmatrix} + \lambda e \begin{bmatrix}
0 \\
\frac{1}{\partial U/\partial x_2} - \frac{1}{u}
\end{bmatrix} u
\]

\( \{S, U\}_J \) is the thermodynamic driving force

\[
\{S, U\}_J = T_1 - T_2 = \frac{\partial S}{\partial x}^\top J \frac{\partial U}{\partial x} = \left[ \frac{1}{1} \right]^\top \left[ \begin{array}{cc}
0 & -1 \\
1 & 0
\end{array} \right] \left[ \begin{array}{c}
T_1 \\
T_2
\end{array} \right]
\]

Hence, \( R(x, T) = \lambda \left( \frac{1}{T_2} - \frac{1}{T_1} \right) = \frac{\lambda}{T_1 T_2} (T_1 - T_2), \) with \( \gamma > 0 \)
The continuous stirred tank reactor (CSTR)

The chemical reaction is denoted by

\[ \nu_1 A_1 + \ldots + \nu_{m-1} A_{m-1} \rightleftharpoons \nu_m A_m, \]

\( \nu_1, \ldots, \nu_m : \) stoichiometric coefficients
\( A_1, \ldots, A_m : \) chemical species

together with the definition of the reaction rate:

\[ r(A, T) = r_f(A_f, T) - r_r(A_f, T) \]

with \( A \) the affinity of reaction.

The mathematical model

The balance equations [Aris, 1989],

\[ \dot{n}_i = F_{ei} - F_{si} + r_i V, \]

\( \dot{S} = \sum_{i=1}^{m} (F_{ei} s_{ei} - F_{si} s_i) + \frac{Q}{T_e} + \sigma, \)

with \( n_i \) number of moles, \( V \) volume, \( F_{ei}, F_{si} \) molar flows, \( s_{ei}, s_i \) molar entropies, \( T_w \) jacket temperature and \( Q \) the heat flux.
The continuous stirred tank reactor (CSTR)

The chemical reaction is denoted by

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together with the definition of the reaction rate:

\[ r(A, T) = r_f(A_f, T) - r_r(A_f, T) \]

with \( A \) the affinity of reaction.

The CSTR may be expressed as IPHS with \( U = \) the internal energy

\[
J = \begin{bmatrix}
0 & \ldots & 0 & \tilde{\nu}_1 \\
0 & \ldots & 0 & \vdots \\
0 & \ldots & 0 & \tilde{\nu}_m \\
-\tilde{\nu}_1 & \ldots & -\tilde{\nu}_m & 0
\end{bmatrix},
\]

\( J \) is the reactions driving force, the affinity of reaction \( A \)

\[
g_1 = \begin{bmatrix}
\nu e - n_f \\
\phi(x, \frac{\partial U}{\partial x})
\end{bmatrix},
\]

\[
g_2 = \begin{bmatrix}
0 \\
\frac{1}{T}
\end{bmatrix},
\]

\[
\begin{bmatrix}
u_1 \\ u_2
\end{bmatrix} = \begin{bmatrix}
\frac{F}{V} \\
T_e
\end{bmatrix}
\]

\( \{S, U\}_J = A = -\sum_{i=1}^{m} \tilde{\nu}_i \mu_i \)

\( \gamma = \frac{rV}{TA} \geq 0, \)

\( \mu_1, \ldots, \mu_m : \) chemical potentials

\( rV : \) molar flow
Energy based availability function

Stability and stabilization
Energy based availability function

The availability function

- Proposed by A. Alonso and E. Ydstie
- The “classical approach” uses the total entropy as convex extension to construct the availability function using thermodynamic considerations.

Consider Gibb’s relation

\[ dU = TdS - PdV + \sum_{i=1}^{N-2} \mu_idn_i = w(z)^\top dz. \]

With \( z = [S, V, n_1, \ldots, n_{N-2}]^\top \) and \( w(z) = [T(z), -P(z), \mu_1(z), \ldots, \mu_{N-2}(z)] \) the vectors of extensive and intensive. \( U \) is a homogeneous function of degree 1, so from Euler’s Theorem,

\[ U = w(z)^\top z, \quad w(z) = \frac{\partial U}{\partial z}(z) \]

The energy based availability function

\[ A(x, x^*) = U(x) - \left[ U(x^*) + \frac{\partial U}{\partial x}(x^*)^\top (x - x^*) \right] \geq 0 \]

where \( x^* \) is a reference and possibly a desired steady state.
Stabilization

Proposition

The closed-loop equilibrium $x^*$ of a controlled IPHS is asymptotically stable if $A$ is strictly convex and $x^*$ satisfies:

$$\gamma \{S, U\} J \{A, U\} - \left(\frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*)\right)^T gu \geq 0,$$

with strict equality only at $x^*$, $u^*$, where $u^*$ is the steady state value of the control-input at the desired equilibrium.

$$\frac{dA}{dt} = \left(\frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*)\right)^T \frac{dx}{dt}$$

$$= -R \left(\frac{\partial U}{\partial x}(x)^T J \frac{\partial U}{\partial x}(x)\right) + \left(\frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*)\right)^T g(u), \quad \text{Def. IPHS}$$

$$= -\gamma \{S, U\} J \{A, U\} + \left(\frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*)\right)^T g(u), \quad \text{Def. Poisson Br}$$

Since $\gamma > 0$ and the availability $A$ qualifies as a Lyapunov function, the system is stable if the relation holds. Asymptotic stability follows invoking La Salle’s invariance principle on a region around $x^*$. 

H. Ramírez et. al. (TFMST’13)
Energy based availability function

Examples: The heat exchanger and the CSTR

The heat exchanger

**Constant mass** → A qualifies as Lyapunov function

\[ T^* \] is the desired temperature

Applying the previous Proposition

\[
\gamma T^*(T_1 - T_2)^2 + (T^* - T_2) \left( \frac{u - T_2}{uT_2} \right) \geq 0,
\]

\[
(\gamma T^* T_2(T_1 - T_2)^2 + T^* - T_2) u - T_2(T^* - T_2) \geq 0.
\]

The closed-loop system will converge asymptotically to the the desired steady state \( T^* > 0 \) if the control input is selected such that the previous equation is greater than zero for all \( T \neq T^* \).

Simplest choice is

\[ u = T^* \]
The CSTR

Applying the previous Proposition (Constant volume $\rightarrow A$ qualifies as Lyapunov function)

$$
= \left( \frac{rV}{T.A} \right) \left( T \sum_{i=1}^{m} \bar{v}_i \mu_i^* - T^* \sum_{i=1}^{m} \bar{v}_i \mu_i \right) A - \left( \frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*) \right) ^\top (g_1 u_1 + g_2(u_2))
$$

$$
= \left( \frac{rV}{T.A} \right) ( - T A^* + T^* A ) A - \left( \frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*) \right) ^\top (g_1 u_1 + g_2(u_2))
$$

In steady state: $A^* = \sum_{i=1}^{m} \bar{v}_i \mu_i^* = 0$ and $T^* > 0$

Stab. Cond. $\Rightarrow \left( \frac{rV}{T.A} \right) T^* A^2 - \left( \frac{\partial U}{\partial x}(x) - \frac{\partial U}{\partial x}(x^*) \right) ^\top (g_1 u_1 + g_2(u_2)) \geq 0$

Select $u_1$ and $u_2$ such that

$$
- \left[ (\mu - \mu^*) ^\top (n_e - n) + (T - T^*) \phi \left( x, \frac{\partial U}{\partial x} \right) \right] u_1 - (T - T^*) \frac{\lambda(u_2 - T)}{T} \geq 0
$$

One possibility

$$
u_1 = - (\mu - \mu^*) ^\top (n_e - n) - (T - T^*) \phi \left( x, \frac{\partial U}{\partial x} \right),$$

$$u_2 = T^*,$$
Final remarks

- IPHS have been used to derive a class of PBC for irreversible thermodynamic systems.
- An energy based availability function has been defined and used as Lyapunov function for IPHS.
- The approach has been used for PBC of irreversible processes in an analogous manner as PBC techniques of mechanical systems.

Ongoing work

IPHS description and control of chemical reaction networks (D. Sbarbaro)


Final remarks and future work

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