Dissipation and Invariance in Process Networks
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Aim: Understand the idea of invariance in passive control systems
Passivity Based Control

Control system:

\[
\frac{dx}{dt} = f(x) + g(x, u)
\]

control system

\[
y = h(x)
\]

observations

Example: MD with thermostat

\[
\dot{r}_i = v_i + \chi r_i
\]

strain

\[
\dot{v}_i = \frac{F(r_i)}{m_i} + \chi v_i - \alpha v_i
\]

friction

\[
\dot{V} = 3V \chi
\]
Definitions:

\[ u \xrightarrow{S} y \]

Storage Function: \( V : x \rightarrow \mathbb{R}^{+/0} \)

\[
\frac{dV}{dt} \leq u^T y - \beta \|\zeta\|_2^2, \text{ passive (dissipative) if } \beta \geq 0
\]

\( \beta > 0 \)

- Input strictly passive if \( \zeta \rightarrow u \)
- Output strictly passive if \( \zeta \rightarrow y \)
- State strictly passive if \( \zeta \rightarrow x \)

\[
\frac{dV}{dt} = u^T y, \quad \text{Lossless (Hamiltonian, } V \text{ is "Invariant"})
\]
Passivity Theorem (Input-Output Theory)

A Feedback connection of a passive/lossless system \( S \) and a strictly input passive control system \( C \) is finite gain stable.

\[
u = g_0 e, \quad \text{strictly input passive if } g_0 > 0
\]
Proof

\[ \frac{dV}{dt} \leq (u + n_2)y - \beta \zeta^2, \quad \text{control system} \]

\[ \frac{dW}{dt} \leq (-y + n_1)u - g_0 e^2 \quad \text{controller} \]

\[ \frac{d(V + W)}{dt} \leq \begin{pmatrix} n_1 \\ n_2 \end{pmatrix}^T \begin{pmatrix} y \\ u \end{pmatrix} - g_0 e^2 - \beta \zeta^2, \quad \text{closed loop system is passive} \]
Passivity via Classical Thermodynamics

Classical System: Macro State $Z(x) = (U, V, N_1, ..., N_{nc}, A, Q_e, ..)$

\[
Z_1 + Z_2 = Z_3
\]

$U(Z_3) = U(Z_1) + U(Z_2)$, First Law

$S(Z_3) \geq S(Z_1) + S(Z_2)$, Second Law

Assumption: There exists an entropy function $S(Z)$ which is $C^1$, concave and homogeneous degree one.

\[
S(Z) = k_B \ln \Omega(U, V, N)
\]

\[
\ln(\Omega_1 + \Omega_2) = \ln(\Omega_1) + \ln(\Omega_2)
\]

\[
\Omega(U, V, N) = \frac{\mathcal{E}}{\hbar^{3N}} \int \delta(U - H(p^{3N}, q^{3N})) dp^{3N} dq^{3N}
\]
\[ A = w_1^T Z - S(Z) \geq 0 \]

\[ w_1 = \frac{\partial S}{\partial Z} \bigg|_{Z=Z_1} \]

\[ Z = (U, V, M_1, ..., M_M) \]

\[ w = (1, -P, -\mu_1, ..., -\mu_{nc}, \sigma, V, ...) \beta, \quad \beta = T^{-1} \]

Gibbs: \( Z_1 \) and \( Z_2 \) in equilibrium iff \( A = 0 \iff w_1 = w_2 \)
Passivity of Classical Non-Equilibrium Systems

\[ \frac{dZ}{dt} = -L(w_1 - w) + u, \quad L > 0 \]

Very large reservoir \( Z_1 \)

\[ \frac{dA}{dt} = (w_1 - w)^T \frac{dZ}{dt} \]

\[ = -(w_1 - w)^T L(w_1 - w) + (w_1 - w)^T (u - u_1) \]

\[ \text{dissipation} \quad \text{control} \]

\[ u = u_1 - K(w_1 - w), \quad K > 0 \]
Process Networks

Graph: $G = (P, F)$

Each node is a process system (Conservation laws hold)
\[
\frac{dZ_i}{dt} = \sum_{i=1}^{n_i} f_{ij} + p_i \quad \text{“Kirchoff Current Law”}
\]

\[
\sum_{i=1}^{n_f} X_i = 0, \quad X_i = w_i - w_j \quad \text{“Kirchoff Voltage Law”}
\]

“Tellegen Theorem” (power balance)

\[
0 = \sum_{\text{ports}} \tilde{f}_j^T \tilde{w}_i - \sum_{\text{storage}} \tilde{w}^T \frac{d\tilde{Z}}{dt} - \sum_{\text{internal flows}} \tilde{X}_i^T \tilde{f}_i - \sum_{\text{source/sink}} \tilde{p}_k^T \tilde{w}_k
\]

Duality pairing, vector spaces \(P=(f,p,dZ/dt)\) and \(D=(X,w,w)\) are orthogonal
\[ A = (w_1 - w)^T (Z_1 - Z) \geq 0, \quad \frac{dA}{dt} = \tilde{w}^T \frac{d\tilde{Z}}{dt} \]

Classical Irrev Thermo \( \tilde{p}_k^T \tilde{w}_k \geq 0, f = LX, L > 0 \)

\[
\frac{dA}{dt} = \sum \tilde{f}_j^T \tilde{w}_i - \sum \tilde{X}_i^T L_i \tilde{X}_i - \sum \tilde{p}_k^T \tilde{w}_k
\]

Theorem: Classical non-equilibrium systems (Linear laws) are passive.

Stable stationary states exist (Prigogine) when boundary conditions are fixed.
Generalization of CIT

Entropy: \( S = w^T Z \geq 0 \)

\[
\frac{dS}{dt} = \sum_{\text{ports}} f_j^T w_i - \sum_{\text{flows}} X_i^T f - \sum_{\text{source/sink}} p_k^T w_k
\]

Assumption: Suppose entropy production is convex and homogeneous degree 1

Positive deviations: \( \tilde{X}^T \tilde{f} + \tilde{w}^T \tilde{p} \geq 0 \)

1. Stable stationary states exist provided boundary control is passive
2. Entropy production is minimized (Euler-Lagrange System)
3. Relaxation possible by balancing flow dissipation vs rx
Invariants and Inventory Control

\[ E(Z_3) = E(Z_1) + E(Z_2), \quad \text{First Law (convex)} \]

\[
\frac{dE}{dt} = \sum_{\text{ports}} f_j^T \eta_i - \sum_{\text{flows}} X_i^T f - \sum_{\text{source/sink}} p_k^T \eta_k
\]

"Energy production" \( \omega(f, p) = 0 \)

Electrical energy converted to heat
Potential energy converted to kinetic energy
.....

Hamitonian /Positive Real/Lossless/Conservative
Inventory Control

\[ \frac{dE}{dt} = \sum_{\text{ports}} f_j^T \eta_i = g(Z,u), \quad \text{supply rate} \]

Mapping: \( \phi(Z,u) \rightarrow E^* - E \), is passive

\[ g(Z,u) = -K(E - E^*) + \frac{dE^*}{dt}, \quad \text{"High Gain Control"} \]
How can the system be dissipative and lossless at the same time?

\[ A(Z) = -(w_1 - w)^T (Z_1 - Z) \geq 0 \]
\[ E(Z) = (\eta_1 - \eta)^T (Z_1 - Z) \geq 0 \]

Depending on the point of view - neither \( E(Z) \) nor \( S(Z) \) are positive definite on \( Z \) (Gibbs etc).

A question of observables - Dissipativity is an input output property
Modification to Storage function

\[ W(Z) = \underbrace{A(Z)}_{\text{Dissipative on } \tilde{w}} + \frac{1}{2} \sum_{\text{phases}} \tilde{E}(Z)^2 + \text{other invariants?} \geq 0 \]

\[ \frac{dW}{dt} = \sum_{\text{ports}} \tilde{f}_j^T \tilde{w}_i - \sum_{\text{flows}} \tilde{X}_i^T L_i \tilde{X}_i - \sum_{\text{source/sink}} \tilde{p}_k^T \tilde{w}_k + \sum_{\text{phases}} \tilde{E}\phi \]

- Lossless, needs control to stay on manifold E*
- Boundary control
- Dissipative component
- Source/sink may be dissipative
- Lossless/Hamiltonian inventory control
Other Invariants in Chemistry (103 of them)

Los Alamos National Laboratory Chemistry Division

Periodic Table of the Elements

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Carbothermic Aluminum
D. Roha O Fortini (Alcoa), Yuan Xu, Mohit Aggarwal, Balaji Sukumar

Challenges:
Multiphase CFD, turbulence
1 gas phase
2 fluid phases
2++ solid phases
50+ compounds
Electric potentials
Turbulence
5 invariants $Z = (\text{Al}, \text{C}, \text{O}, \text{U}, \text{V})$

Issues:
System Design
Stability
Optimization (kg/kW)

Vapor pressure
$P/\text{Pa}$ 1 10 100 1 k 10 k 100 k
at $T/\text{K}$ 1482 1632 1817 2054 2364 2790

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Aluminum atom mole balance

\[ F_{\text{Al}}^{\text{in}} + 2F_{\text{Al}_2\text{O}_3}^{\text{in}} + 2F_{\text{C}_3\text{Al}_2\text{O}_3}^{\text{in}} = F_{\text{Al}_4\text{C}_3}^{\text{out}} + 2F_{\text{Al}_2\text{O}_3}^{\text{out}} + 4F_{\text{Al}_4\text{C}_3}^{\text{out}} \]  

(1)

Carbon atom mole balance

\[ F_{\text{C}_3}^{\text{in}} + F_{\text{CO}_2}^{\text{in}} = F_{\text{C}_3}^{\text{out}} + F_{\text{CO}_2}^{\text{out}} + 3F_{\text{Al}_4\text{C}_3}^{\text{out}} \]  

(2)

Oxygen atom mole balance

\[ F_{\text{Al}_2\text{O}_3}^{\text{in}} + F_{\text{CO}_2}^{\text{in}} + 3F_{\text{Al}_2\text{O}_3}^{\text{in}} = F_{\text{Al}_2\text{O}_3}^{\text{out}} + F_{\text{CO}_2}^{\text{out}} \]  

(3)

% Recovery of Al metal

- 100%
- 80%
- 60%
- 40%
- 20%

Mole Fraction of Al\(_4\)C\(_3\)

- Simulation
- Design Relation with 75% Recovery

Kg flow of gas / Kg flow of carbon
The structure of thermodynamics and Control
Luiz Felipe Tavares (March 21, 2003)

Input-Output theory
- Clausius Kelvin Theory
- Efficiency of reversible processes
- Carnot Caratheodory
- Finite Time Thermodynamics
- Efficiency of irreversible processes
- Berry, Salamon, Andresen

Thermodynamics
- Gibbs Theory
- Stability of equilibrium states
- Tisza, Callen
- Irreversible thermodynamics
- Stability of steady states close to equilibrium
- Onsager, Prigogine, Glansdorff

Internal Stability
- Passivity theory
- Input-output operators
- Desoer, Willems
- Stability theory
- Stability of "equilibrium" states
- Lyapunov, Kalman, ..