Dissipation and Invariance in Process Networks

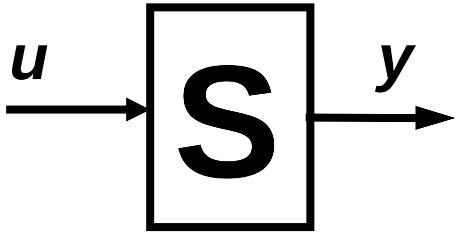
B. Erik Ydstie
Carnegie Mellon

Mohit Aggarwal, Yuan Xu, Michael Wartman

Aim: Understand the idea of invariance in passive control systems

Passivity Based Control

Control system:



$$\frac{dx}{dt} = f(x) + g(x,u) \qquad \text{control system}$$

$$y = h(x) \qquad \text{observations}$$

Example: MD with thermostat

strain

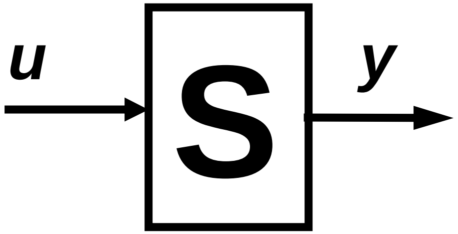
friction

$$\dot{r}_i = v_i + \chi r_i$$

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

$$\dot{V} = 3V\chi$$

Definitions:



Storage Function: $V : \mathrm{x} \rightarrow \mathrm{R}^{+/0}$

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

$\beta > 0$

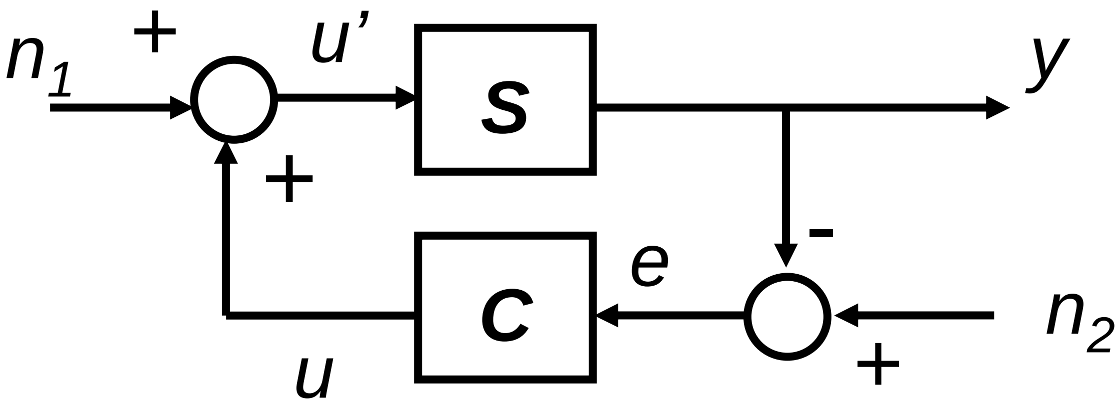
Input strictly passive if $\varsigma \rightarrow u$

Output strictly passive if $\varsigma \rightarrow y$

State strictly passive if $\varsigma \rightarrow \mathrm{x}$

$$\frac{dV}{dt} = u^T y, \quad \text{Lossless (Hamiltonian, } V \text{ is "Invariant")}$$

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

$$\frac{dV}{dt} \le (u + n_2) y - \beta \varsigma^2, \qquad \text{control system}$$

$$\frac{dW}{dt} \le (-y + n_1) u - g_0 e^2 \qquad \text{controller}$$

$$\frac{d(V+W)}{dt} \le \begin{pmatrix} n_1 \\ n_2 \end{pmatrix}^T \begin{pmatrix} y \\ u \end{pmatrix} - g_0 e^2 - \beta \varsigma^2, \qquad \text{closed loop system is passive}$$

Passivity via Classical Thermodynamics

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

$$\boxed{Z_1} + \boxed{Z_2} = \boxed{Z_3}$$

$$U(Z_3)=U(Z_1)+U(Z_2),\quad \text{First Law}$$

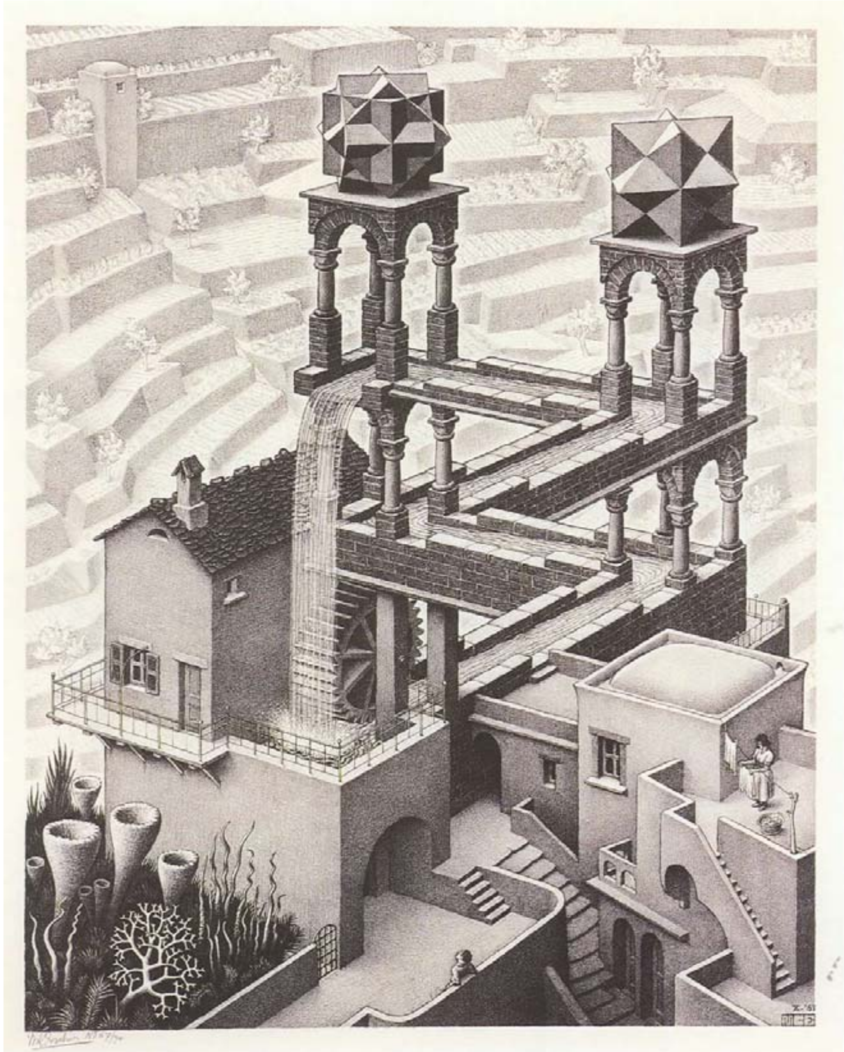
$$S(Z_3)\geq S(Z_1)+S(Z_2),\quad \text{Second Law}$$

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

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

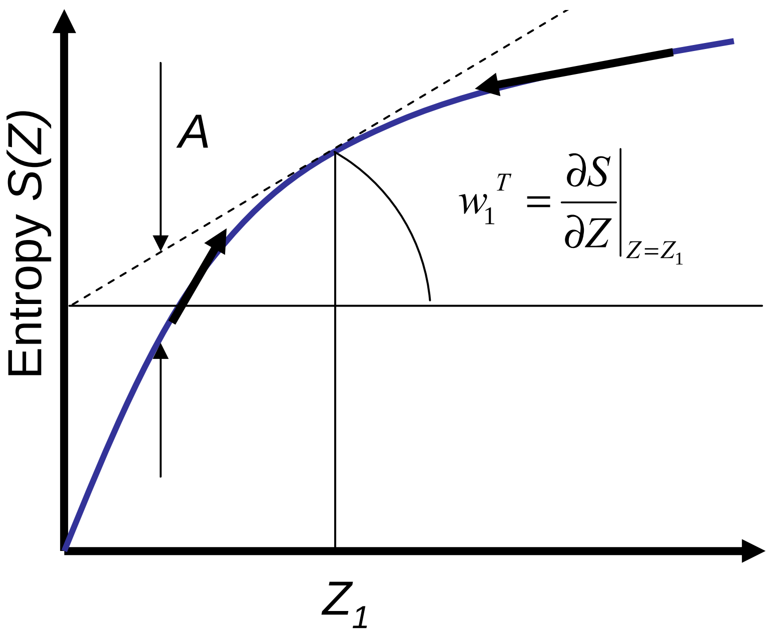
$$\ln(\Omega_1+\Omega_2)=\ln(\Omega_1)+\ln(\Omega_2)$$

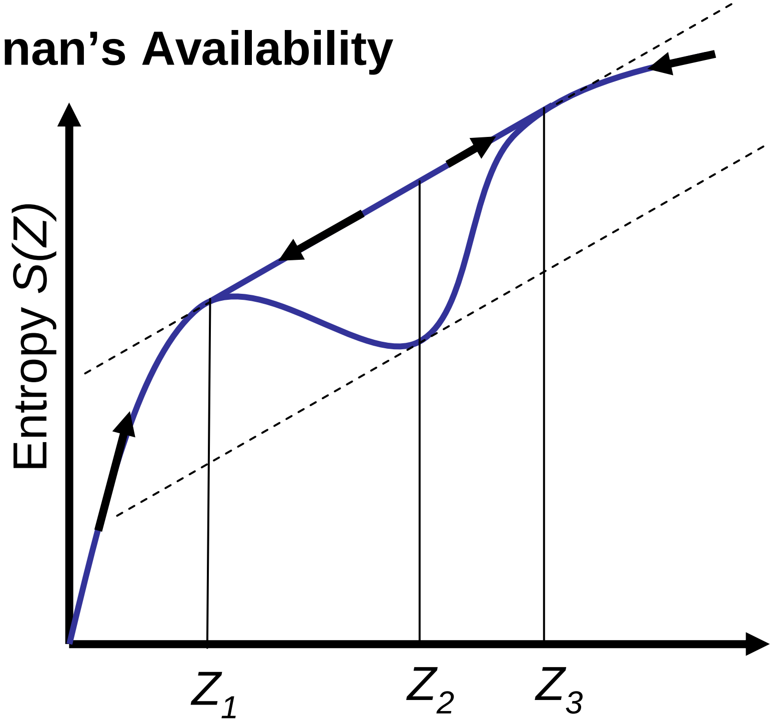
$$\Omega(U,V,N)=\frac{\varepsilon}{\hbar^{3N}N!}\int\delta(U-H(p^{3N},q^{3N}))dp^{3N}dq^{3N}$$



$$A = w_1^T Z - S(Z) \geq 0$$

Keenan's Availability



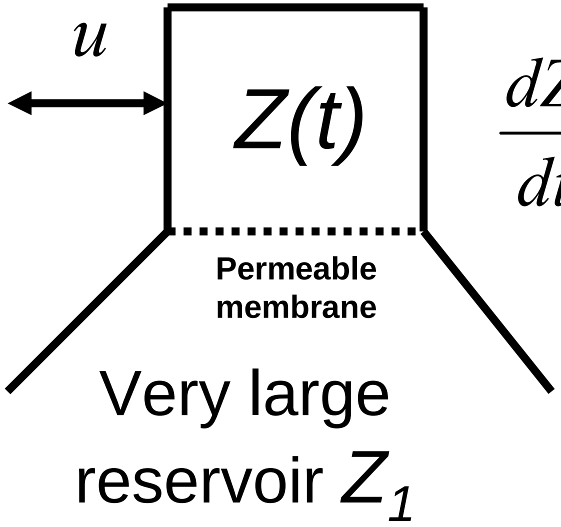


$$Z = (U, V, M_1, \ldots, M_1)$$

$$w = (1, -P, -\mu_1, \ldots, \mu_{nc}, \sigma, V, \ldots)\beta, \qquad \beta = T^{-1}$$

Gibbs: Z_1 and Z_2 in equilibrium iff $A = 0 \Leftrightarrow w_1 = w_2$

Passivity of Classical Non-Equilibrium Systems



$$\frac{dZ}{dt} = -\mathrm{L}(w_1 - w) + u, \qquad \mathrm{L} > 0$$

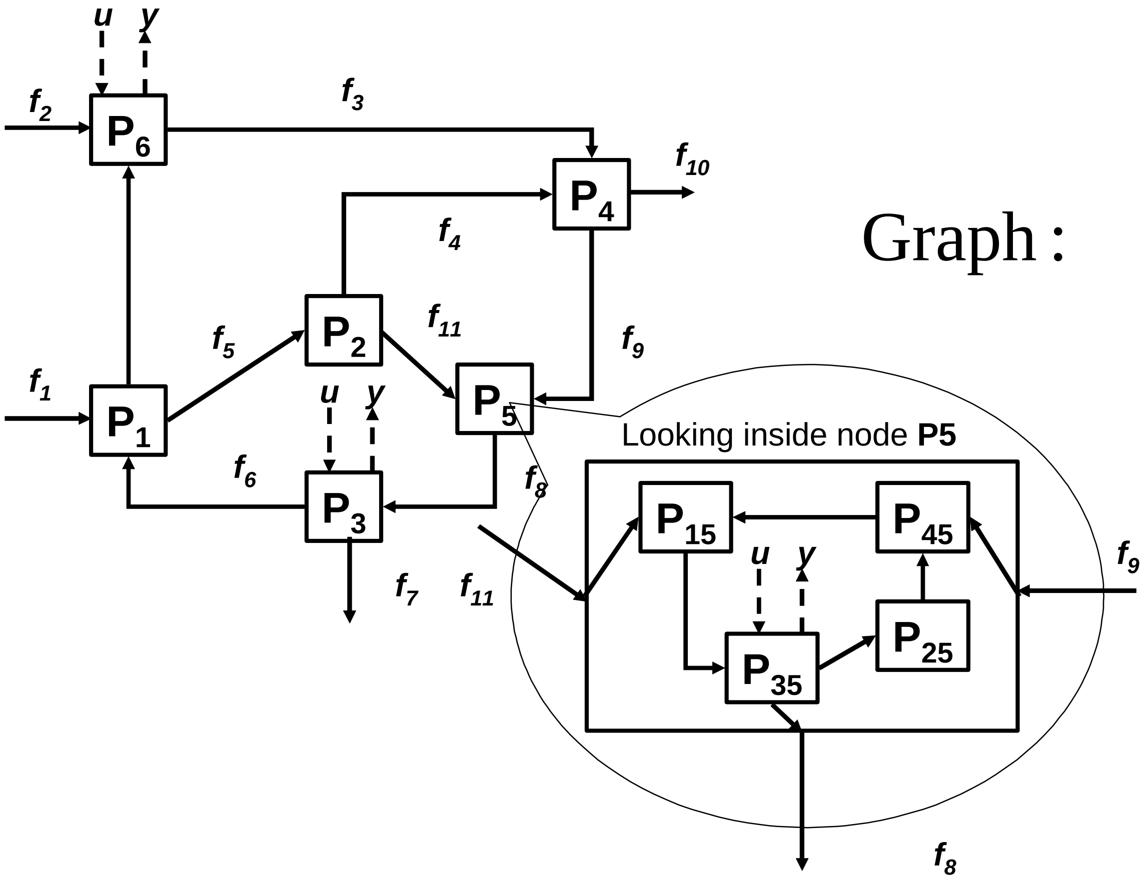
Fourier
Fick
Newton
Ohm

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

$$= \underbrace{-(w_1 - w)^T \mathrm{L}(w_1 - w)}_{\textbf{dissipation}} + \underbrace{(w_1 - w)^T (u - u_1)}_{\textbf{control}}$$

$$u = u_1 - K(w_1 - w), \qquad K > 0$$

Process Networks



$$\text{Graph}: \quad G = (P, F)$$

Each node is a process system (Conservation laws hold)

$$\frac{dZ_i}{dt} = \sum_{i=1}^{n_i} f_{ij} + p_i$$

"Kirchoff Current Law"

$$\sum_{i=1}^{n_f} X_i = 0, \qquad X_i = w_i - w_j$$

"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 $\tilde{p}_k^{\ T} \tilde{w}_k 0 \geq 0,\ f = LX, L > 0$

$$\frac{dA}{dt} = \underbrace{\sum_{\text{ports}} \tilde{f}_j^{\ T} \tilde{w}_i}_{\text{boundary control}} - \underbrace{\sum_{\text{flows}} \tilde{X}_i^{\ T} \mathrm{L}_i \tilde{X}_i}_{\text{dissipation}} - \underbrace{\sum_{\text{source/sink}} \tilde{p}_k^{\ T} \tilde{w}_k}_{\text{reaction}}$$

$$\tilde{f}_{boundary} \to u$$
$$\tilde{w}_{boundary} \to y$$
$$w_{nodes} \to \varsigma$$

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

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

Generalization of CIT

$$\text{Entropy}: \qquad S = w^T Z \geq 0$$

$$\frac{dS}{dt} = \underbrace{\sum_{\text{ports}} f_j^{\,T} w_i}_{\text{boundary control}} \; \underbrace{- \sum_{\text{flows}} X_i^{\,T} f - \sum_{\text{source/sink}} p_k^{\,T} w_k}_{\text{Entropy production} \quad \sigma(f,p) \geq 0}$$

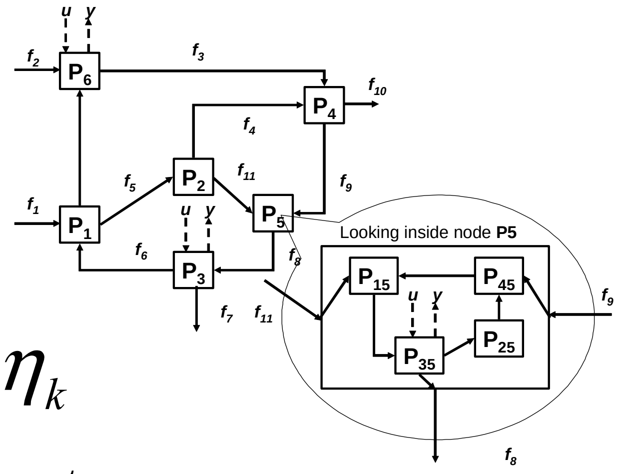
Assumption: Suppose entropy production is convex and homogeneous degree 1

$$\text{Positive deviations}: \qquad \tilde{X}^T \tilde{f} + \tilde{w}^T \tilde{p} \geq 0$$

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

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



$$\frac{dE}{dt} = \underbrace{\sum_{\text{ports}} f_j^{\,T} \eta_i}_{\text{boundary control}} \; \underbrace{- \sum_{\text{flows}} \mathrm{X}_i^{\,T} f - \sum_{\text{source/sink}} p_k^{\,T} \eta_k}_{\text{"Energy production"} \quad \omega(f,p)=0}$$

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

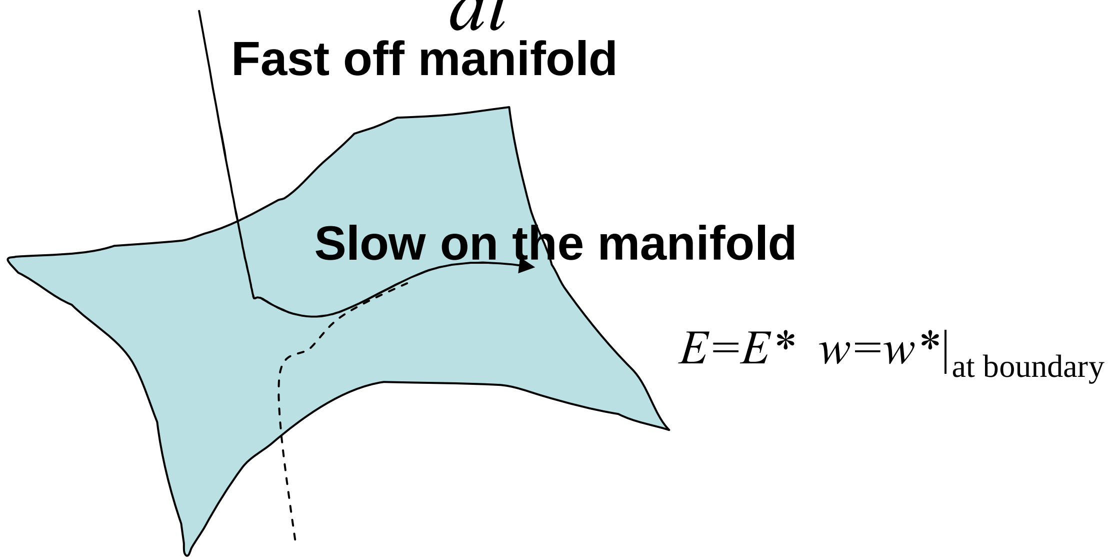
Hamitonian /Positive Real/Lossless/Conservative

Inventory Control

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

$$\text{Mapping} : \phi(Z,u) \to E^* - E, \quad \text{is passive}$$

$$g(Z,u) = -K(E - E^*) + \frac{dE^*}{dt}, \quad \text{"High Gain Control"}$$

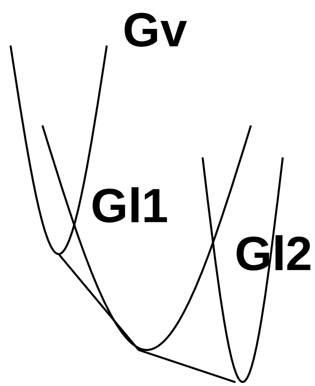


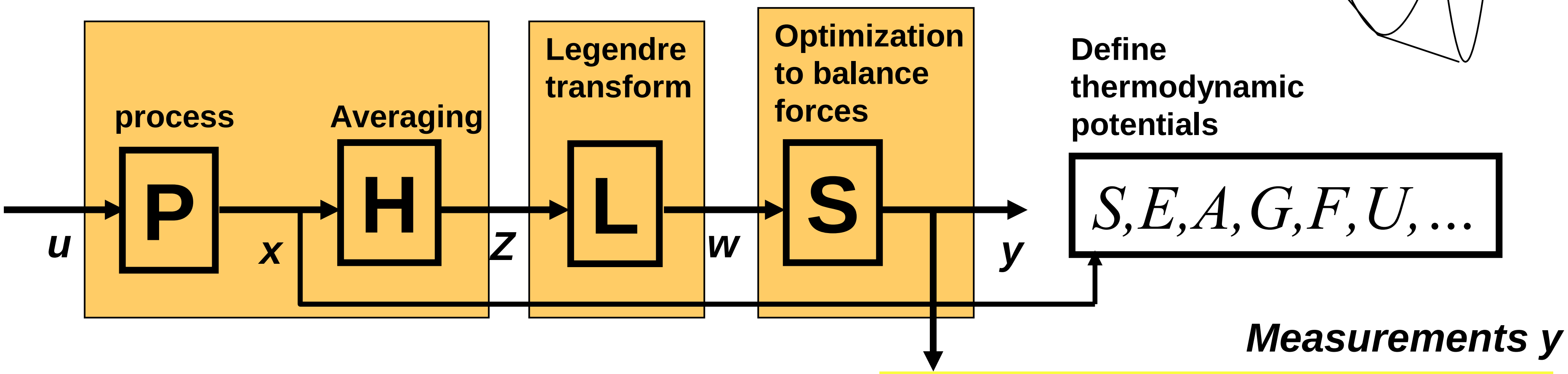
How can the system be dissipative and lossless at the same time?

$$A(Z) = -(w_1 - w)^T (Z_1 - Z) \geq 0$$

$$E(Z) = (\eta_1 - \eta)^T (Z_1 - Z) \geq 0$$

Convex Hull Is C1





phases, conformations, molecular structure, temp pressure,voltage, surface tension,…
MANY coordinates

Gibbs-Duhem: $dw^T Z = 0$

Depends on the point of view

-neither *E(Z)* nor *S(Z)* are positive definite on Z (Gibbs etc).

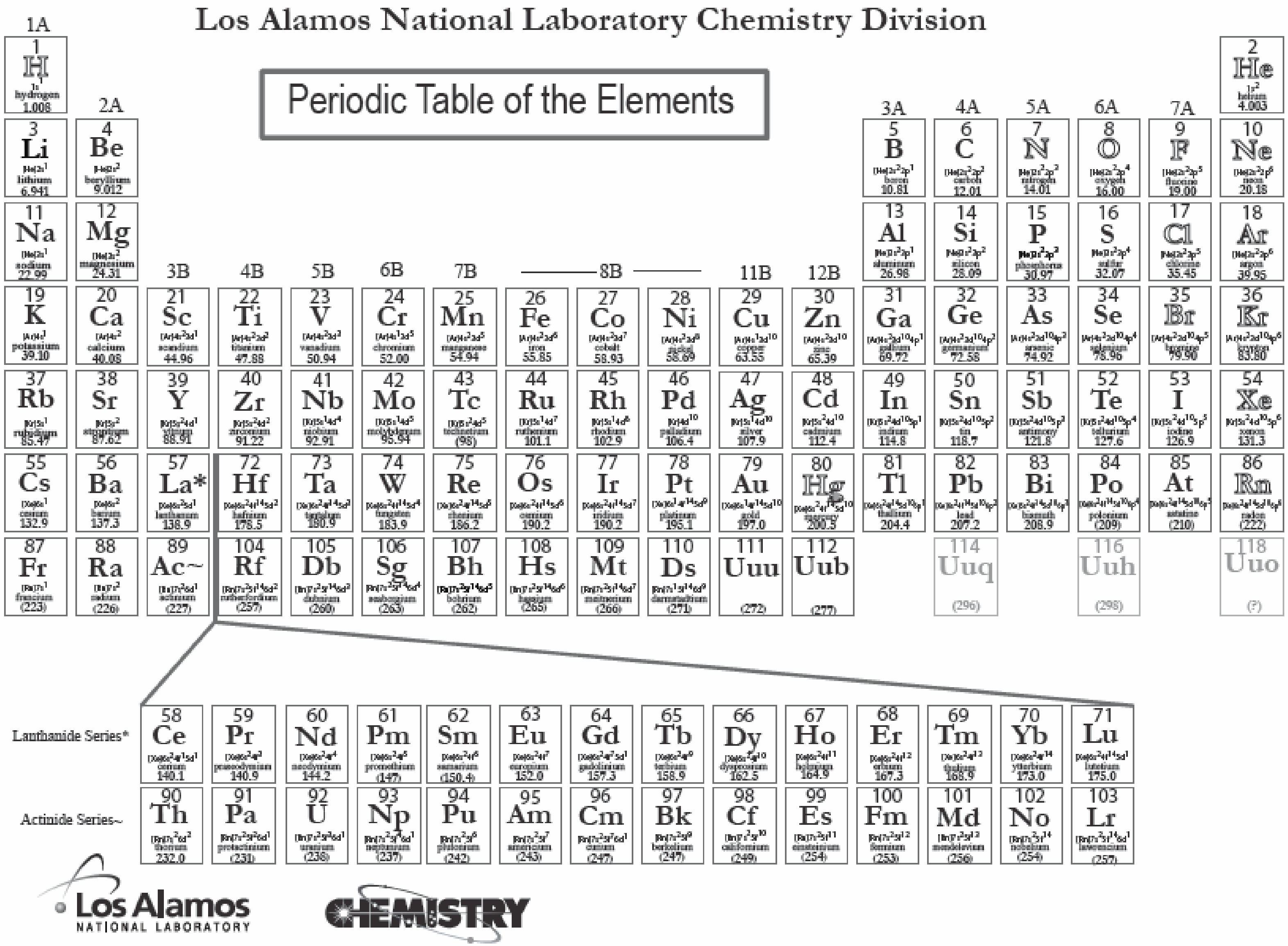
A question of observables - Dissipativity is an input output property

Modification to Storage function

$$W(Z) = \underbrace{A(Z)}_{\text{Dissipative on } \tilde{w}} + \underbrace{\frac{1}{2}\sum_{\text{phases}} \tilde{E}(Z)^2 + \text{other invariants?}}_{\text{Lossless, needs control to stay on manifold E*}} \geq 0$$

$$\frac{dW}{dt} = \underbrace{\sum_{\text{ports}} \tilde{f}_j^{\,T} \tilde{w}_i}_{\text{boundary control}} - \underbrace{\sum_{\text{flows}} \tilde{X}_i^{\,T} \mathrm{L}_i \tilde{X}_i}_{\text{dissipative component}} - \underbrace{\sum_{\text{source/sink}} \tilde{p}_k^{\,T} \tilde{w}_k}_{\text{reaction maybe dissipative}} + \underbrace{\sum_{\text{phases}} \tilde{E}\phi}_{\text{Lossless/Hamiltonian inventory control}}$$

Other Invariants in Chemistry (103 of them)

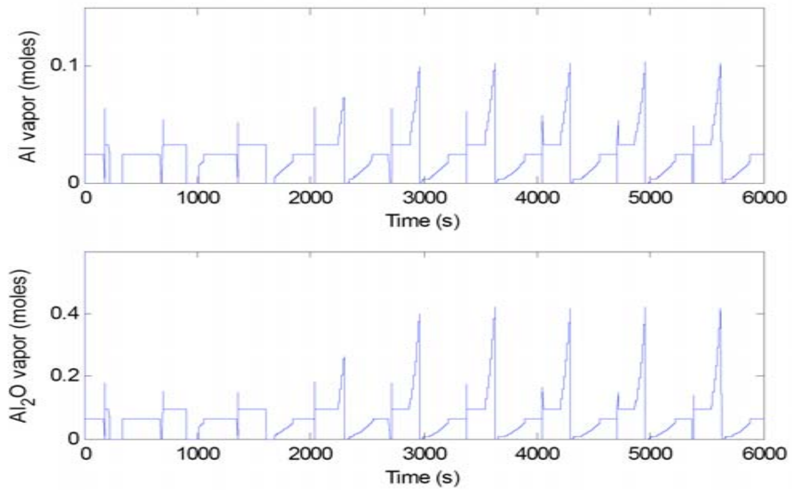


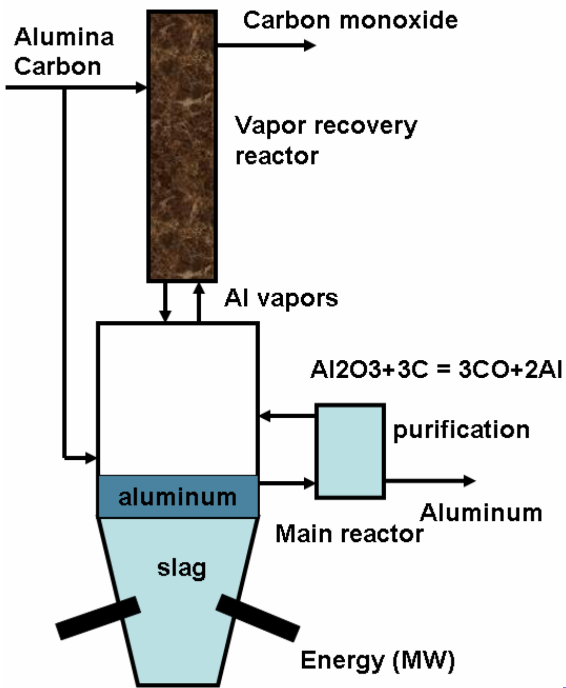
Carbothermic Aluminum

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

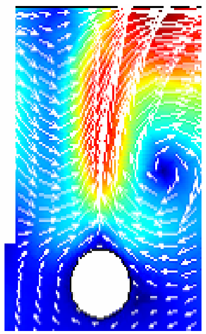
Vapor pressure

P/Pa	1	10	100	1 k	10 k	100 k
at *T*/K	1482	1632	1817	2054	2364	2790

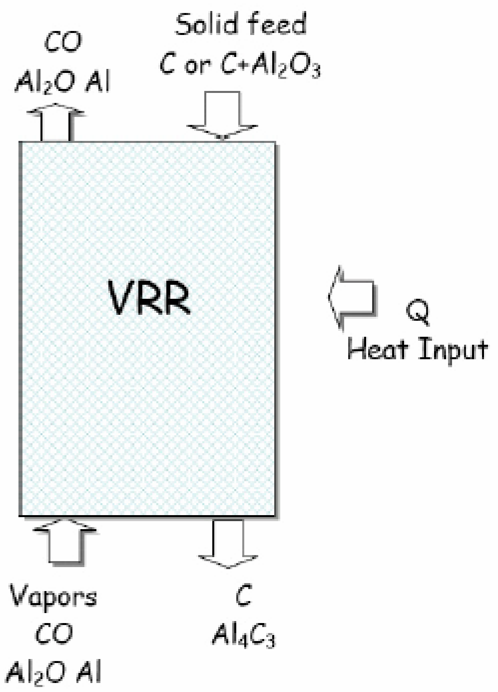




ssues:
System Design
Stability
Optimization (kg/kW)



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



Aluminum atom mole balance

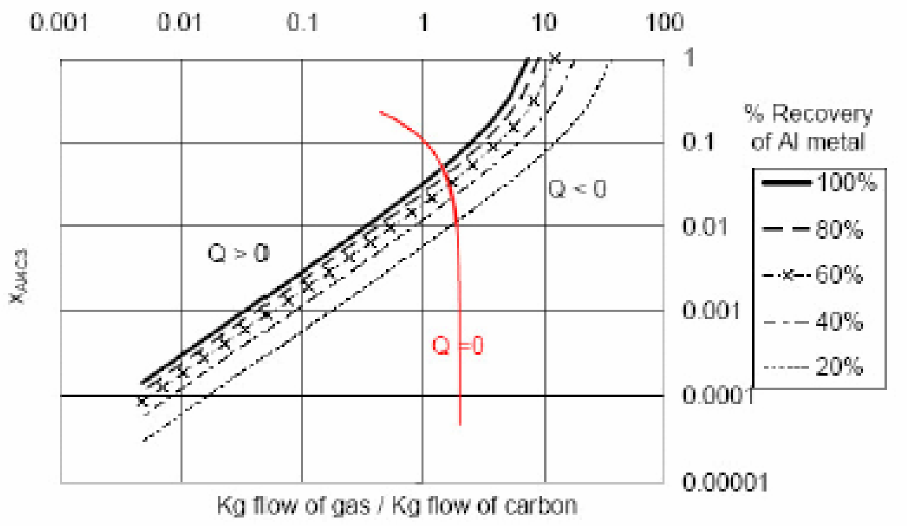
$$F^{in}_{Al_g} + 2F^{in}_{Al_2O_g} + 2F^{in}_{Al_2O_{3s}} = F^{out}_{Al_g} + 2F^{out}_{Al_2O_g} + 4F^{out}_{Al_4C_{3s}} \quad (1)$$

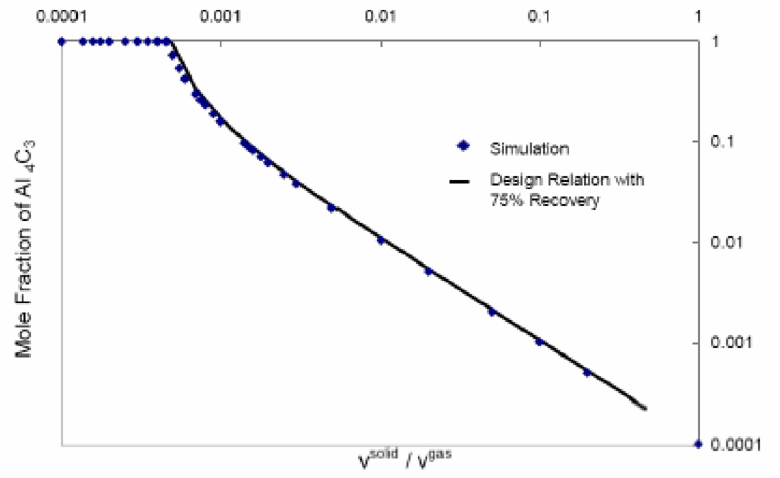
Carbon atom mole balance

$$F^{in}_{C_s} + F^{in}_{CO_g} = F^{out}_{C_s} + F^{out}_{CO_g} + 3F^{out}_{Al_4C_{3s}} \quad (2)$$

Oxygen atom mole balance

$$F^{in}_{Al_2O_g} + F^{in}_{CO_g} + 3F^{in}_{Al_2O_{3s}} = F^{out}_{Al_2O_g} + F^{out}_{CO_g} \quad (3)$$





The structure of thermodynamics and Control

Luiz Felipe Tavares (March 21, 2003)