

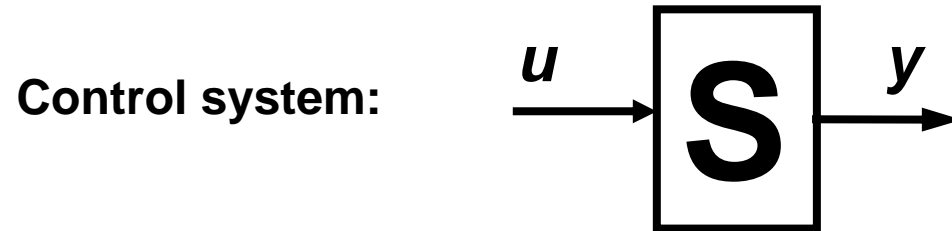
Dissipation and Invariance in Process Networks

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Aim: Understand the idea of invariance in passive control systems

Passivity Based Control

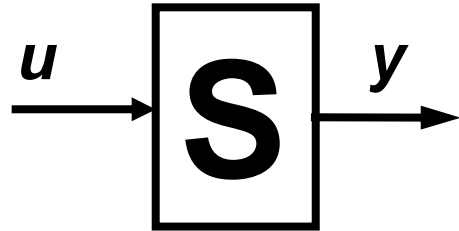


$$\begin{aligned} \frac{dx}{dt} &= f(x) + g(x, u) && \text{control system} \\ y &= h(x) && \text{observations} \end{aligned}$$

Example: MD with thermostat

$$\begin{aligned} \dot{r}_i &= v_i + \chi r_i && \text{strain} \\ \dot{v}_i &= \frac{F(r_i)}{m_i} + \chi v_i - \alpha v_i && \text{friction} \\ \dot{V} &= 3V\chi \end{aligned}$$

Definitions:



Storage Function : $V : \mathbf{x} \rightarrow \mathbb{R}^{+/\circ}$

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

$\beta > 0$

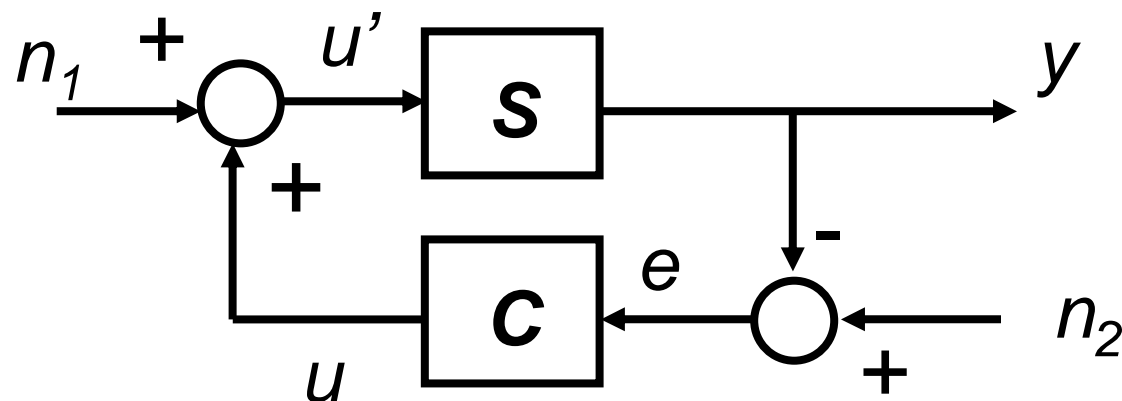
Input strictly passive if $\zeta \rightarrow u$

Output strictly passive if $\zeta \rightarrow y$

State strictly passive if $\zeta \rightarrow \mathbf{x}$

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

Passivity Theorem (Input-Output Theory)



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

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

Proof

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

$$\frac{dW}{dt} \leq (-y + n_1)u - g_0e^2 \quad \text{controller}$$

$$\frac{d(V + W)}{dt} \leq \begin{pmatrix} n_1 \\ n_2 \end{pmatrix}^T \begin{pmatrix} y \\ u \end{pmatrix} - g_0e^2 - \beta\zeta^2, \quad \text{closed loop system is passive}$$

Passivity via Classical Thermodynamics

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

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

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

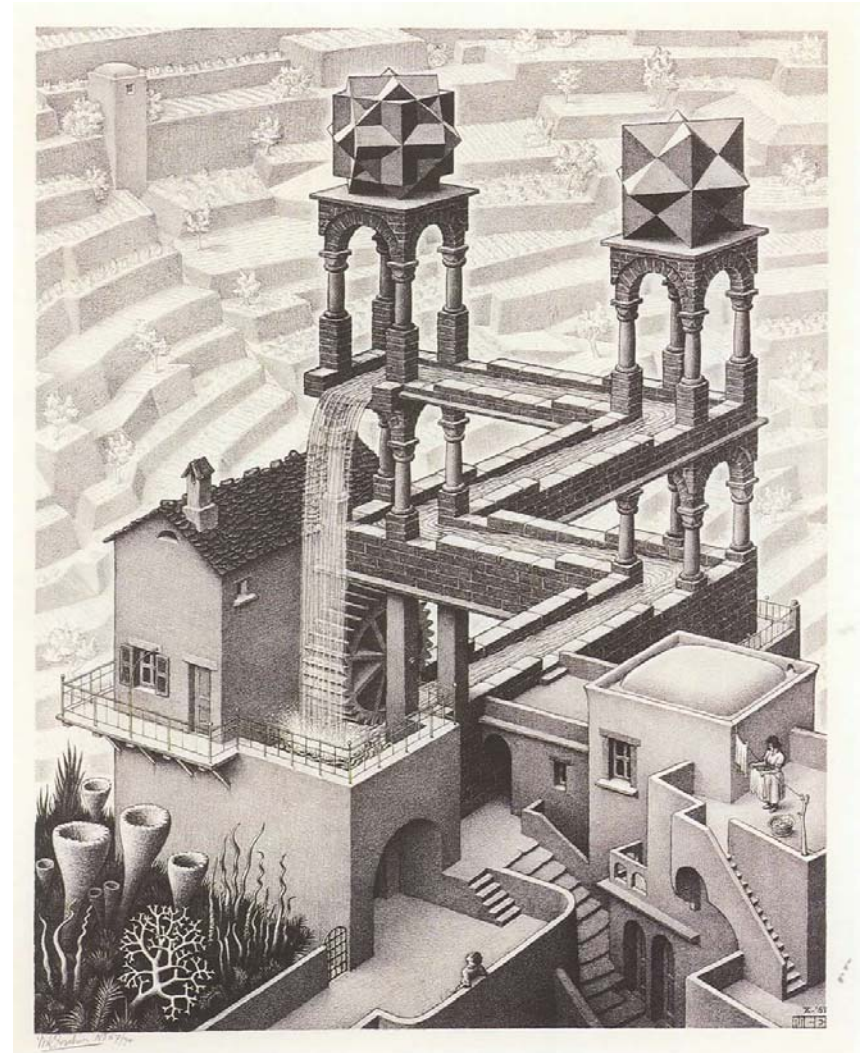
$S(Z_3) \geq S(Z_1) + S(Z_2)$, Second Law

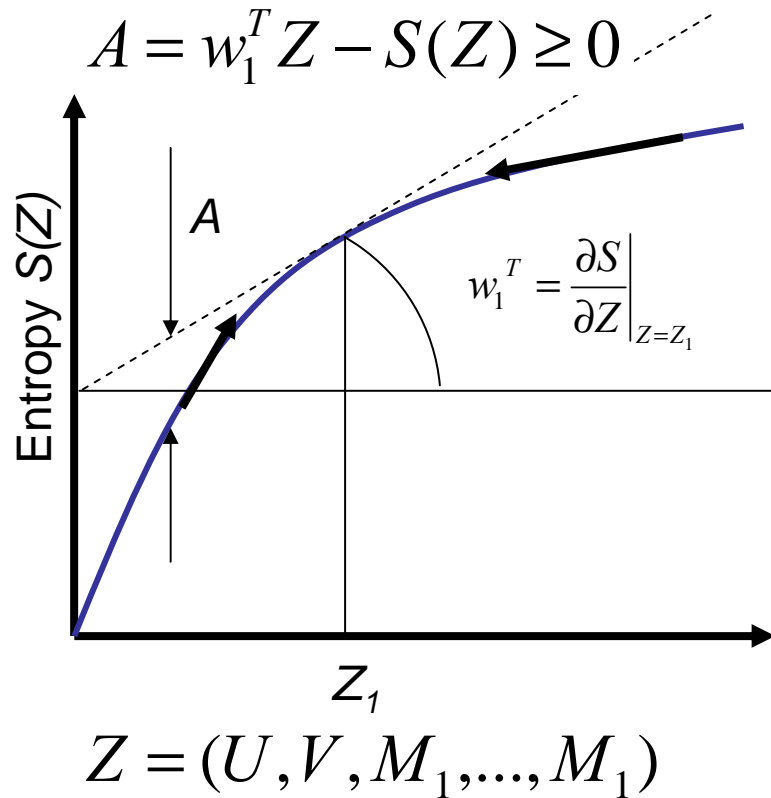
Assumption: There exists an entropy function $S(Z)$ which is C^1 , concave and homogeneous degree one.

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

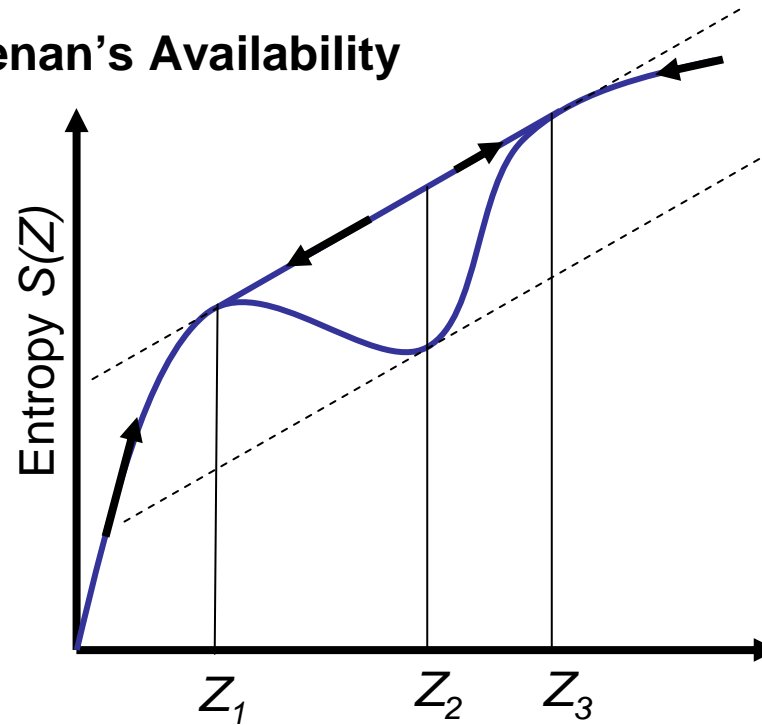
$$\ln(\Omega_1 + \Omega_2) = \ln(\Omega_1) + \ln(\Omega_2)$$

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





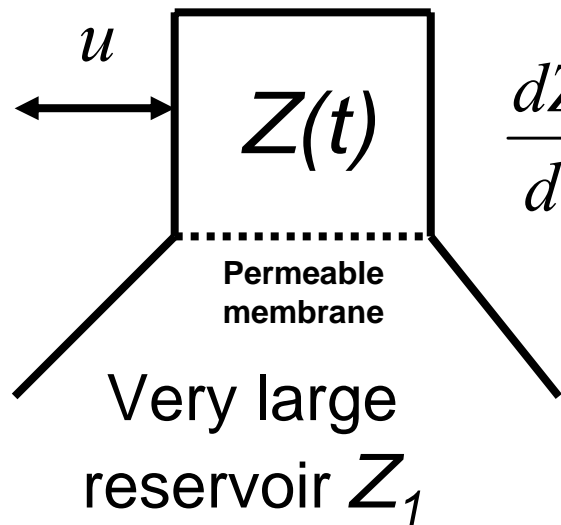
Keenan's Availability



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

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

Passivity of Classical Non-Equilibrium Systems



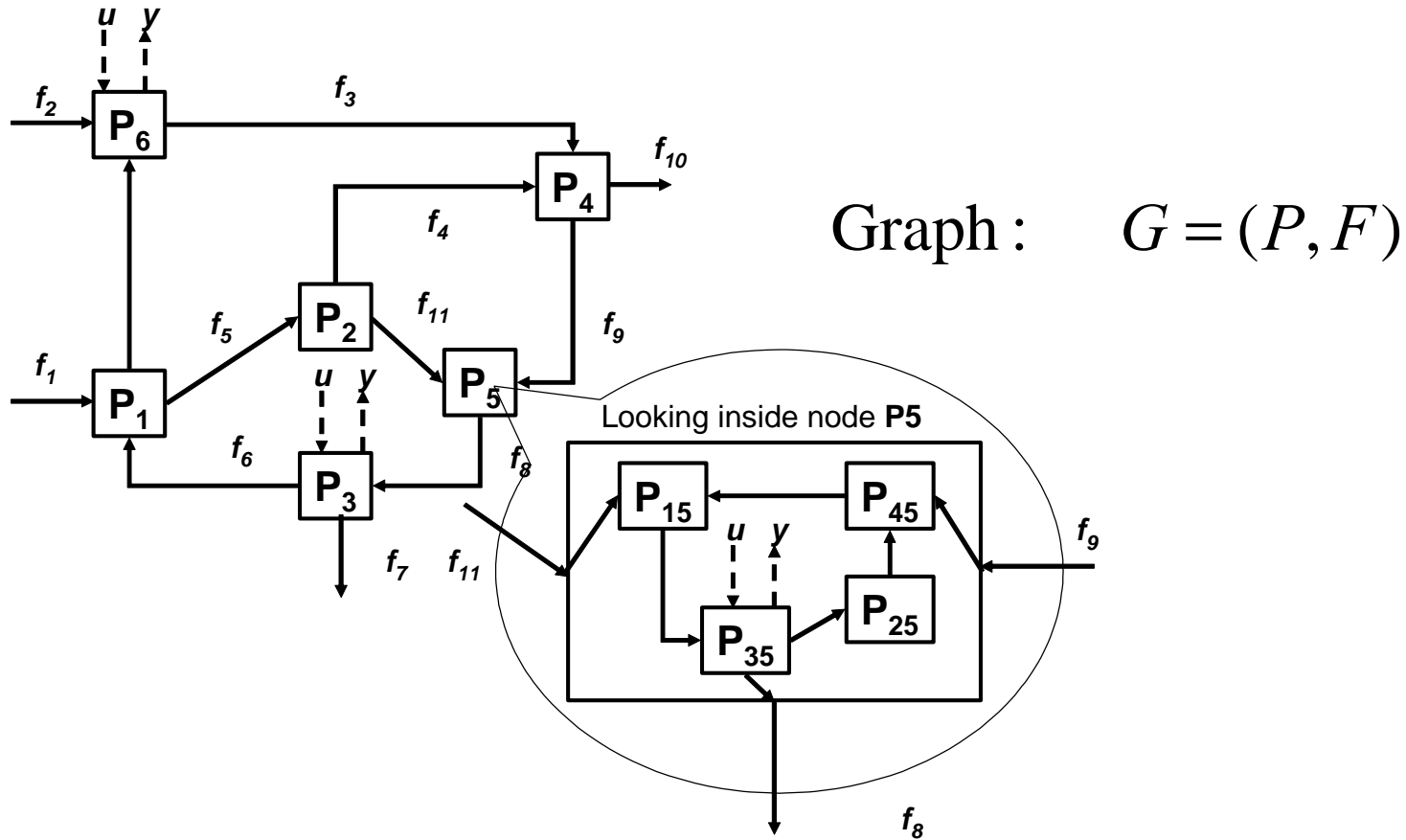
$$\frac{dZ}{dt} = -L(w_1 - w) + u, \quad L > 0$$

Fourier
Fick
Newton
Ohm

$$\begin{aligned} \frac{dA}{dt} &= (w_1 - w)^T \frac{dZ}{dt} \\ &= \underbrace{-(w_1 - w)^T L (w_1 - w)}_{\text{dissipation}} + \underbrace{(w_1 - w)^T (u - u_1)}_{\text{control}} \end{aligned}$$

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

Process Networks



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

$$\frac{dA}{dt} = \underbrace{\sum \tilde{f}_j^T \tilde{w}_i}_{\text{ports}} - \underbrace{\sum \tilde{X}_i^T L_i \tilde{X}_i}_{\text{flows}} - \underbrace{\sum \tilde{p}_k^T \tilde{w}_k}_{\text{source/sink}}$$

boundary control dissipation reaction

$$\tilde{f}_{boundary} \rightarrow u$$

$$\tilde{w}_{boundary} \rightarrow y$$

$$w_{nodes} \rightarrow \zeta$$

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

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

Generalization of CIT

Entropy : $S = w^T Z \geq 0$

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

Assumption: Suppose entropy production is convex and homogeneous degree 1

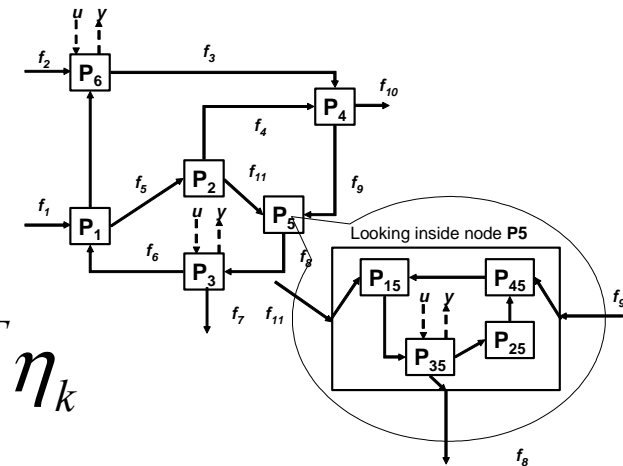
Positive deviations : $\tilde{X}^T \tilde{f} + \tilde{w}^T \tilde{p} \geq 0$

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

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

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



Electrical energy converted to heat
Potential energy converted to kinetic energy

.....

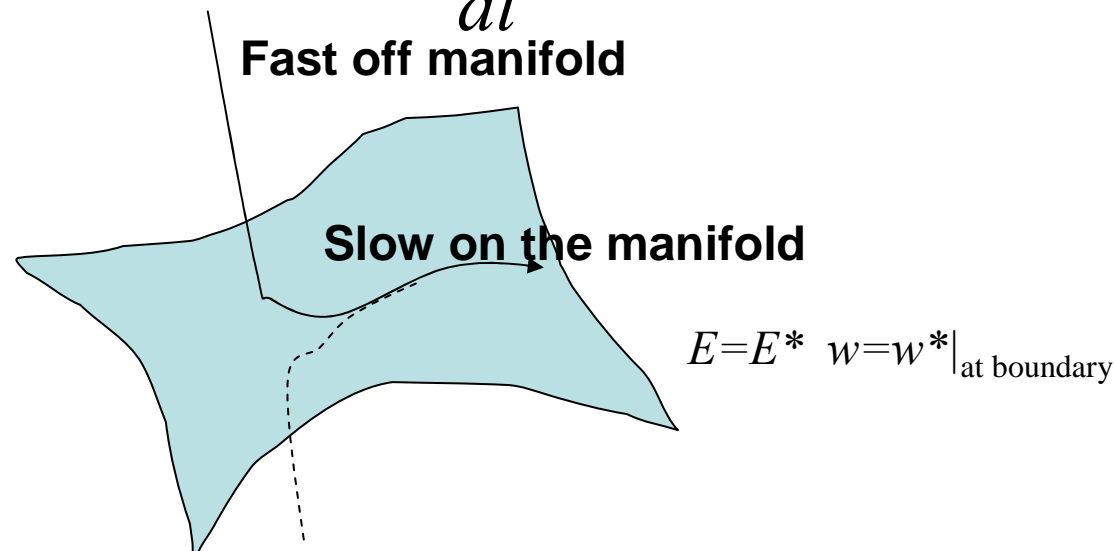
Hamiltonian /Positive Real/Lossless/Conservative

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

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

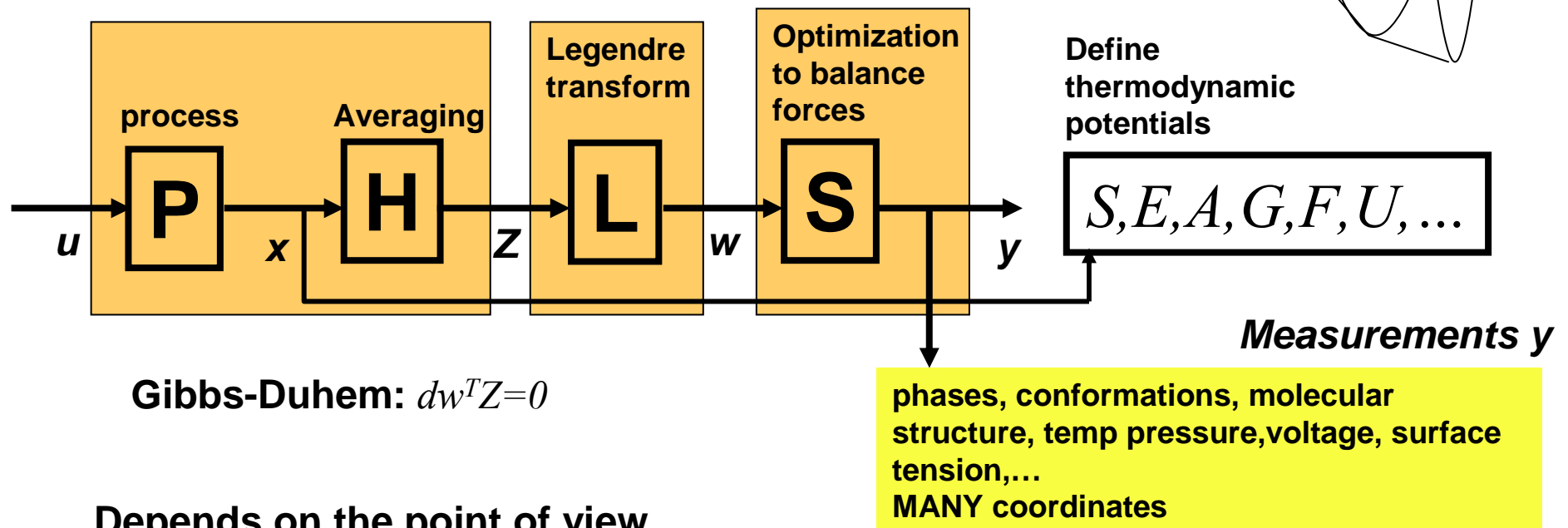
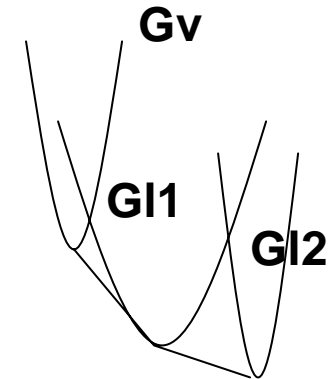


How can the system be dissipative and lossless at the same time?

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

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

Convex Hull
Is C1



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

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

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

Other Invariants in Chemistry (103 of them)

Los Alamos National Laboratory Chemistry Division

Periodic Table of the Elements

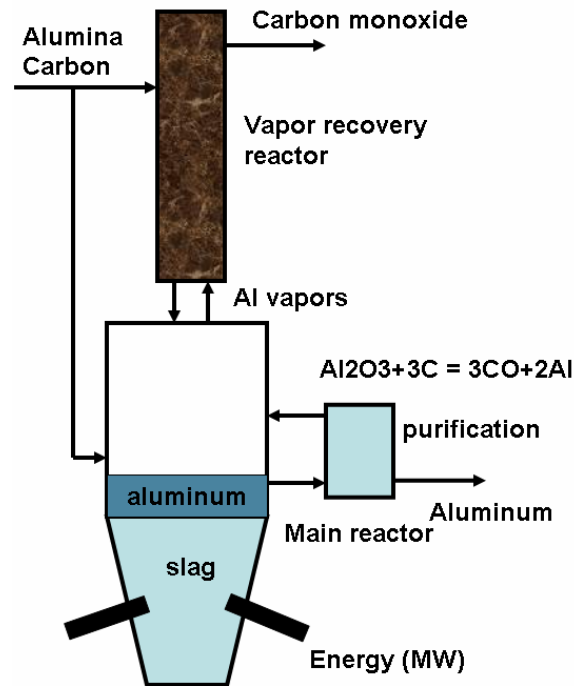
1A	Los Alamos National Laboratory Chemistry Division																2						
1 H hydrogen 1.008																	2 He helium 4.003						
3 Li lithium 6.941	4 Be beryllium 9.012																	5 B boron 10.81	6 C carbon 12.01	7 N nitrogen 14.01	8 O oxygen 16.00	9 F fluorine 19.00	10 Ne neon 20.18
11 Na sodium 22.99	12 Mg magnesium 24.31	3B	4B	5B	6B	7B	8B		11B	12B	13 Al aluminum 26.98	14 Si silicon 28.09	15 P phosphorus 30.97	16 S sulfur 32.07	17 Cl chlorine 35.45	18 Ar argon 39.95							
19 K potassium 39.10	20 Ca calcium 40.08	21 Sc scandium 44.96	22 Ti titanium 47.88	23 V vanadium 50.94	24 Cr chromium 52.00	25 Mn manganese 54.94	26 Fe iron 55.85	27 Co cobalt 58.93	28 Ni nickel 58.69	29 Cu copper 63.55	30 Zn zinc 65.39	31 Ga gallium 69.72	32 Ge germanium 72.58	33 As arsenic 74.92	34 Se selenium 78.96	35 Br bromine 79.90	36 Kr krypton 83.80						
37 Rb rubidium 85.47	38 Sr strontium 87.62	39 Y yttrium 88.91	40 Zr zirconium 91.22	41 Nb niobium 92.91	42 Mo molybdenum 95.94	43 Tc technetium (98)	44 Ru ruthenium 101.1	45 Rh rhodium 102.9	46 Pd palladium 106.4	47 Ag silver 107.9	48 Cd cadmium 112.4	49 In indium 114.8	50 Sn tin 118.7	51 Sb antimony 121.8	52 Te tellurium 127.6	53 I iodine 126.9	54 Xe xenon 131.3						
55 Cs cesium 132.9	56 Ba barium 137.3	57 La* lanthanum 138.9	72 Hf hafnium 178.5	73 Ta tantalum 180.9	74 W tungsten 183.9	75 Re rhenium 186.2	76 Os osmium 190.2	77 Ir iridium 192.2	78 Pt platinum 195.1	79 Au gold 197.0	80 Hg mercury 200.5	81 Tl thallium 204.4	82 Pb lead 207.2	83 Bi bismuth 208.9	84 Po polonium (209)	85 At astatine (210)	86 Rn radon (222)						
87 Fr francium (223)	88 Ra radium (226)	89 Ac~ actinium (227)	104 Rf rutherfordium (261)	105 Db dubnium (262)	106 Sg seaborgium (263)	107 Bh bohrium (264)	108 Hs hassium (265)	109 Mt meitnerium (266)	110 Ds darmstadtium (271)	111 Uuu (272)	112 Uub (277)	114 Uuq (296)	116 Uuh (298)	118 Uuo (?)									
Lanthanide Series*		58 Ce cerium 140.1	59 Pr praseodymium 140.9	60 Nd neodymium 144.2	61 Pm promethium (147)	62 Sm samarium (150.4)	63 Eu europium 152.0	64 Gd gadolinium 157.3	65 Tb terbium 158.9	66 Dy dysprosium 162.5	67 Ho holmium 164.9	68 Er erbium 167.3	69 Tm thulium 168.9	70 Yb ytterbium 173.0	71 Lu lutetium 175.0								
Actinide Series~		90 Th thorium 232.0	91 Pa protactinium (231)	92 U uranium (238)	93 Np neptunium (237)	94 Pu plutonium (242)	95 Am americium (243)	96 Cm curium (247)	97 Bk berkelium (247)	98 Cf californium (249)	99 Es einsteinium (254)	100 Fm fermium (253)	101 Md mendelevium (256)	102 No nobelium (254)	103 Lr lawrencium (257)								

Carbothermic Aluminum

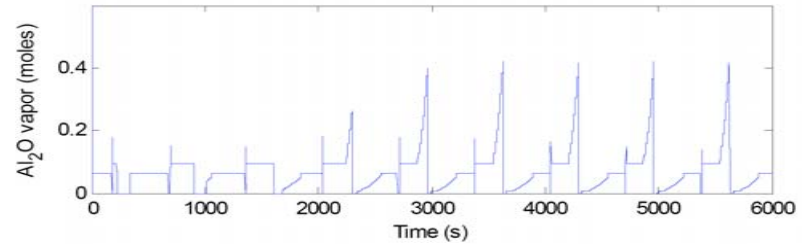
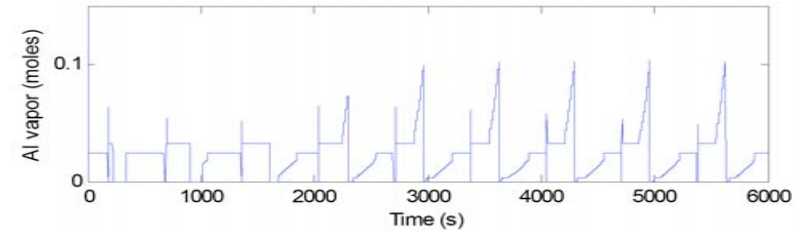
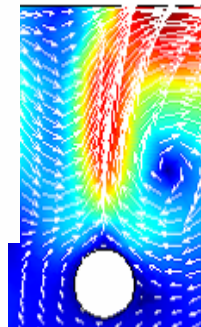
D. Roha O Fortini (Alcoa), Yuan Xu, Mohit Aggarwal, Balaji Sukumar

Vapor pressure

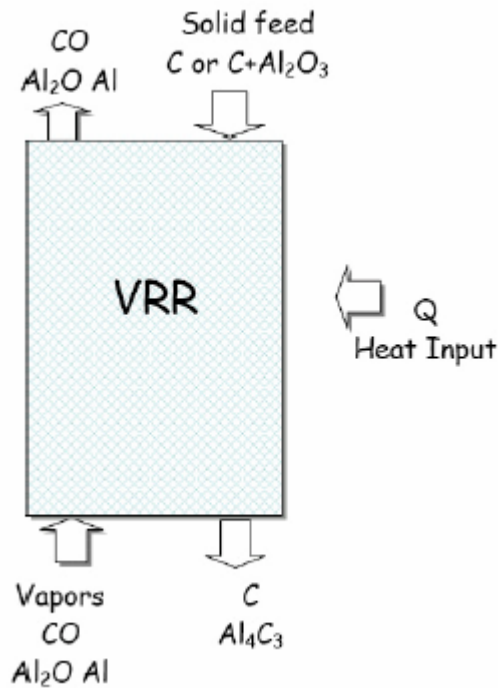
P/Pa	1	10	100	1 k	10 k	100 k
at T/K	1482	1632	1817	2054	2364	2790



Issues:
 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 $Z=(\text{Al}, \text{C}, \text{O}, \text{U}, \text{V})$



Aluminum atom mole balance

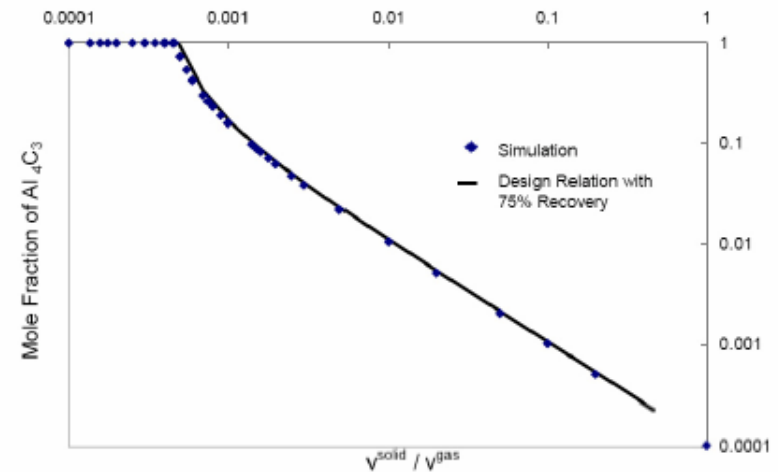
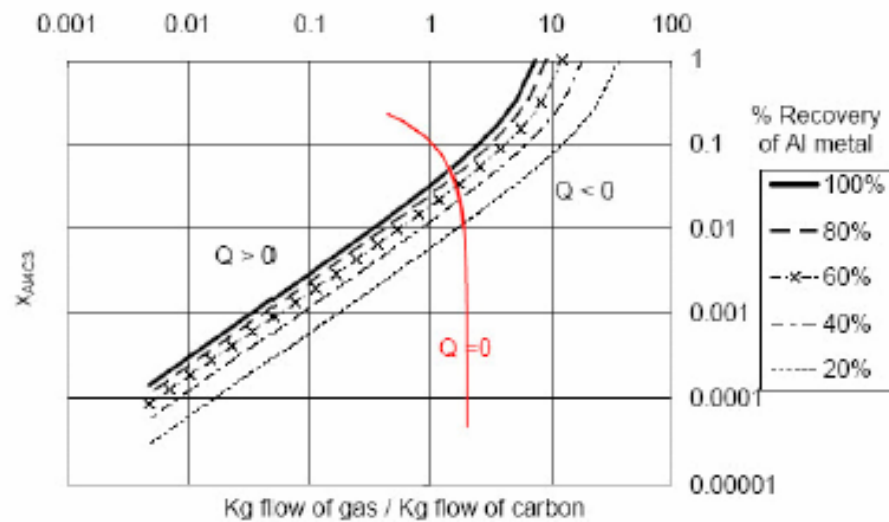
$$F_{Al_2}^{in} + 2F_{Al_2O_3}^{in} + 2F_{Al_2O_{2a}}^{in} = F_{Al_2}^{out} + 2F_{Al_2O_2}^{out} + 4F_{Al_4C_3}^{out} \quad (1)$$

Carbon atom mole balance

$$F_{C_2}^{in} + F_{CO_2}^{in} = F_{C_2}^{out} + F_{CO_2}^{out} + 3F_{Al_4C_3}^{out} \quad (2)$$

Oxygen atom mole balance

$$F_{Al_2O_2}^{in} + F_{CO_2}^{in} + 3F_{Al_2O_{2a}}^{in} = F_{Al_2O_2}^{out} + F_{CO_2}^{out} \quad (3)$$



The structure of thermodynamics and Control

Luiz Felipe Tavares (March 21, 2003)

