MATTER TRANSPORT (CONTINUED)

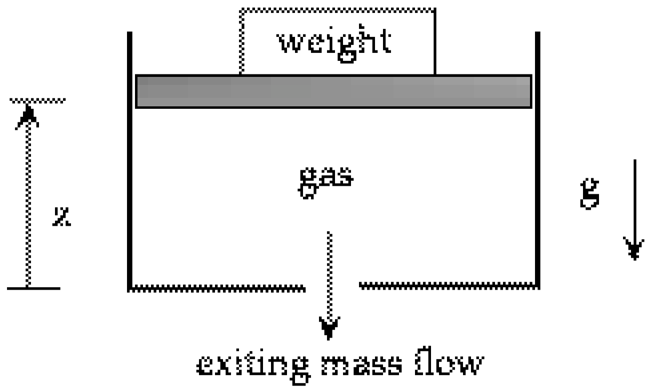
- **There seem to be two ways to identify the effort variable for mass flow**
  - **gradient of the energy function with respect to mass is "matter potential", μ**
  - **— (molar) specific Gibbs free energy**
  - **power dual of mass flow appears to be (molar) specific enthalpy, h**
- **The coupling between mass flow and entropy flow apparently reconciles these**
  - **$h = \mu + Ts$**

CAUTION:

- **Enthalpy is NOT analogous to voltage or force**
  - **it is not always an appropriate power dual for mass flow**

EXAMPLE:

vertically oriented piston & cylinder with exiting mass flow



How do you model the exit flow orifice?

consider kinetic energy transported

Net power flow: consider three terms

flow work rate

internal energy transport rate

kinetic energy transport rate

$$P_{net} = \frac{P}{\rho}\ dN/dt + u\ dN/dt + \frac{v^2}{2}\ dN/dt$$

$$P_{net} = \left(h + \frac{v^2}{2}\right)\ dN/dt$$

Power balance:

subscript c: chamber, t: throat of orifice

$$\left(h_c + \frac{v_c{}^2}{2}\right)\ dN_c/dt = \left(h_t + \frac{v_t{}^2}{2}\right)\ dN_t/dt$$

Mass balance:

$$dN_c/dt = dN_t/dt$$

Assume that velocity at the throat, v_t, is much greater that velocity in the chamber, v_c.

$$v_c << v_t$$

$$\frac{v_c^2}{2} \approx 0$$

$$h_c - h_t = \left(\frac{v_t^2}{2}\right)$$

$$v_t = \sqrt{2\left(h_c - h_t\right)}$$

Mass flow rate

$$dN_t/dt = \rho_t\ A_t\ v_t$$

Thus

$$dN_t/dt = \rho_t\ A_t \sqrt{2\left(h_c - h_t\right)}$$

Does this make physical sense?

Does enthalpy difference drive mass flow?

Snag:

Orifice flow is a typical "throttling" process

Throttling is commonly assumed to occur at constant enthalpy

Assume an ideal gas

$Pv = RT$

$u = c_v T$

$h = u + Pv = (c_v + R)T = c_p T$

Thus enthalpy is proportional to temperature

The model above implies that mass flow is initiated by temperature difference

i.e., it predicts that mass flow must be zero at thermal equilibrium

— NOT TRUE!

WHERE DID WE GO WRONG?

Enthalpy, h, is not an effort in the sense of a gradient that initiates a flow

P_{net} = h dN/dt is a *composite* of distinct power flows

SOLUTION:

model the coupling between components of power flow

ENERGY-BASED APPROACH

IDENTIFY (EQUILIBRIUM) ENERGY STORAGE FUNCTION

variable arguments identify ports

gradients identify efforts

hence P,T,μ for -V,S,N respectively

no dynamics yet

IDENTIFY COUPLING BETWEEN ELEMENTS

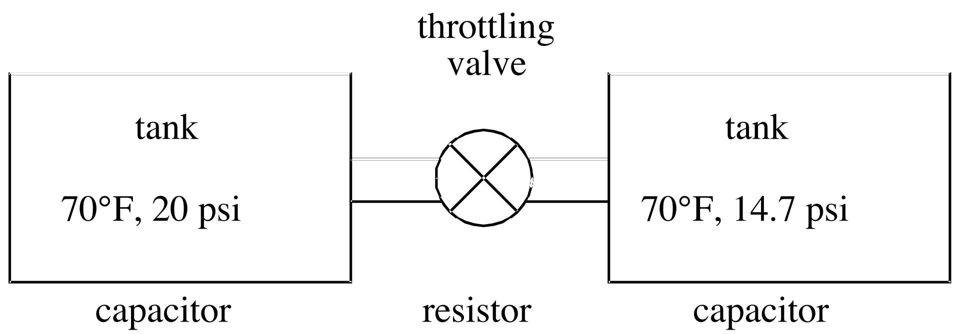
(junction structure)

some coupling may be "embedded" in "dissipation" phenomena

IDENTIFY (STEADY STATE) DISSIPATION FUNCTION

EXAMPLE:

two chambers connected by a throttling valve



Chambers:

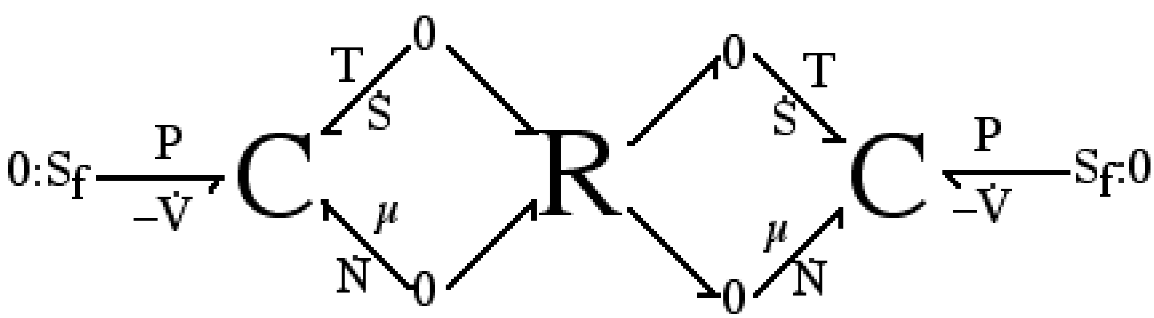
ideal gas

$U_i = m_i c_v T_i = M c_v N_i T_i$

$U_i = (M c_v)\, N_i T_i$

Throttling valve:

a *four-port* resistor R



AN ISSUE:

mass flow is driven by pressure difference

but the pressure-volume port is "closed"

i.e., has no power flow

the capacitors' energy variables (displacements) are

N_1, S_1

N_2, S_2

using energy variables as state variables,

the corresponding inputs to the resistor are efforts

μ_1, T_1

μ_2, T_2

can these resistor inputs properly determine its outputs?

YES:

Gibbs free energy:

$$G = U + PV - TS$$

per unit mass:

$$\mu = u + Pv - Ts$$

$$P = \frac{\mu - u + Ts}{v}$$

$$u = c_v T$$

$$v = V/N$$

$$s = S/N$$

POINT:

Given μ and T and state variables S and N, P can be computed. This formulation would be computationally consistent.

However, it is clumsy and unnecessary.

STEPS IN (NETWORK) MODELING:

formulate the model

choose state variables

formulate equations

choose states:

we care about P and T

both are (invertible) functions of S and N, so could be used as state variables

capacitor pressures

$P_i = \rho_i R T_i$

$\rho_i = N_i / V_i$

a convenient choice of state variables:

N_1, T_1

N_2, T_2

THROTTLING PROCESS:

One crude (but simple) model of a throttling process:

(the model structure is the same for more sophisticated models)

assume flow work is converted into kinetic energy

power balance

$$P_{net} = \left(\frac{P_u}{\rho_u} + \frac{v_u^2}{2}\right) dm_u/dt = \left(\frac{P_t}{\rho_t} + \frac{v_t^2}{2}\right) dm_t/dt$$

subscripts: u, upstream, t, throat

assume no leakage

$$dN_u/dt = dN_t/dt$$

assume negligible upstream velocity

$$v_u << v_t$$

$$\frac{v_t^2}{2} = \left(\frac{P_u}{\rho_u} - \frac{P_t}{\rho_t}\right)$$

$$v_t = \sqrt{2\left(\frac{P_u}{\rho_u} - \frac{P_t}{\rho_t}\right)}$$

volumetric flow rate

$$Q = A_t v_t = A_t\sqrt{2\left(\frac{P_u}{\rho_u} - \frac{P_t}{\rho_t}\right)}$$

mass flow rate

$$dN/dt = \rho_t A_t v_t = \rho_t A_t\sqrt{2\left(\frac{P_u}{\rho_u} - \frac{P_t}{\rho_t}\right)}$$

assume all the flow work goes into speeding up the flow

none into compressing the gas

i.e., assume constant density

$$\rho_u = \rho_t$$

$$dN/dt = \rho_u A_t \sqrt{2\left(\frac{P_u}{\rho_u} - \frac{P_t}{\rho_u}\right)}$$

$$dN/dt = A_t \sqrt{2\rho_u\,(P_u - P_t)}$$

as a result, temperature, specific internal energy and specific enthalpy change

$$\frac{P_u}{P_t} = \frac{T_u}{T_t}$$

if $P_u > P_t$ then $T_u > T_t$

hence $u_u > u_t$

hence $h_u > h_t$

PROBLEM:

throttling is frequently assumed to be isenthalpic

—NO net enthalpy change

SOLUTION:

Assume a mixing and thermal equilibration process to reach a downstream state

Assume that mixing occurs at constant pressure

and proceeds until the net enthalpy change from upstream to downstream is zero.

$P_d = P_t$

$h_d = h_u$

therefore

$T_d = T_u$

therefore

$u_d = u_u$

subscript: d, downstream

The mixing and equilibration process MUST produce entropy

that entropy becomes part of the downstream power flow

—"carried with" the downstream mass flow

There are two distinct components of the net power flow

mass flow

entropy flow

These two flows are coupled

mass flow in and out:

$$dN_u/dt = dN_d/dt = dN/dt = A_t\sqrt{2\rho_u (P_u - P_d)}$$

entropy flow in:

$$dS_u/dt = s_u \, dN/dt$$

entropy flow out:

$$dS_d/dt = s_d \, dN/dt$$

net entropy production rate

$$dS_{net}/dt = dS_d/dt - dS_u/dt = (s_d - s_u) \, dN/dt$$

Is the second law satisfied?

Check the sign of net entropy production:

if $P_u > P_d$

then $dN/dt > 0$

$$s_u - s_o = R \ln \frac{v_u}{v_o} + c_v \ln \frac{T_u}{T_o}$$

subscript o: thermal reference

$$s_u - s_o = R \ln \frac{\rho_o}{\rho_u} + c_v \ln \frac{T_u}{T_o}$$

$$s_d - s_u = R \ln \frac{\rho_u}{\rho_d} + c_v \ln \frac{T_d}{T_u}$$

if the upstream and downstream chambers are at thermal equilibrium

$T_u = T_d$

therefore

$\rho_u > \rho_d$

therefore

$s_d > s_u$

—as required by the second law.

ASIDE:

Note that, for an ideal gas, isenthalpic throttling is only possible if the upstream and downstream temperatures are identical.

In general, upstream and downstream temperatures may differ. The throttling process is no longer isenthalpic, but the model remains valid and consistent with the second law.

Collect resistor equations:

$$dN_u/dt = A_t\sqrt{2\rho_u (P_u - P_d)}$$

$$dN_d/dt = A_t\sqrt{2\rho_u (P_u - P_d)}$$

$$dS_u/dt = s_u\, dN_u/dt$$

$$dS_d/dt = s_d\, dN_d/dt$$

junction equations:

connect four-port resistor to two ports of each capacitor

upstream:

$dS_1/dt = -dS_u/dt$ $\quad$ $dN_1/dt = -dN_u/dt$

$s_u = s_1 = S_1/N_1$ $\quad$ $\rho_u = \rho_1 = N_1/V_1$

$T_u = T_1$ $\quad$ $P_u = P_1 = \rho_u R T_u$

downstream:

$dS_2/dt = dS_d/dt$ $\quad$ $dN_2/dt = dN_d/dt$

$s_d = s_2 = S_2/N_2$ $\quad$ $\rho_d = \rho_2 = N_2/V_2$

$T_d = T_2$ $\quad$ $P_d = P_2 = \rho_d R T_d$

THE FOUR-PORT RESISTOR FUNDAMENTALLY COUPLES MASS FLOWS AND ENTROPY FLOWS

can we display that coupling?

(i.e., where's the modulated transformer we saw before?)

LINEARIZED MODEL:

Consider a formulation in which we compute the pressures from μ and T

$$P = \frac{\mu - u + Ts}{v}$$

based on Gibbs free energy

$$G = U - TS + PV$$

per unit mass:

$$\mu = u - Ts + Pv$$

differentiate

$$d\mu = du - Tds - sdT + Pdv + vdP$$

but per unit mass, u = u(s,v) thus

$$du = Tds - Pdv$$

hence

$$d\mu = vdP - sdT$$

THIS IS A FORM OF THE GIBBS-DUHEM EQUATION

Now approximate the differentials with differences

$$\Delta\mu = \mu_u - \mu_d \approx d\mu$$

$$\Delta P = P_u - P_d \approx dP$$

$$\Delta T = T_u - T_d \approx dT$$

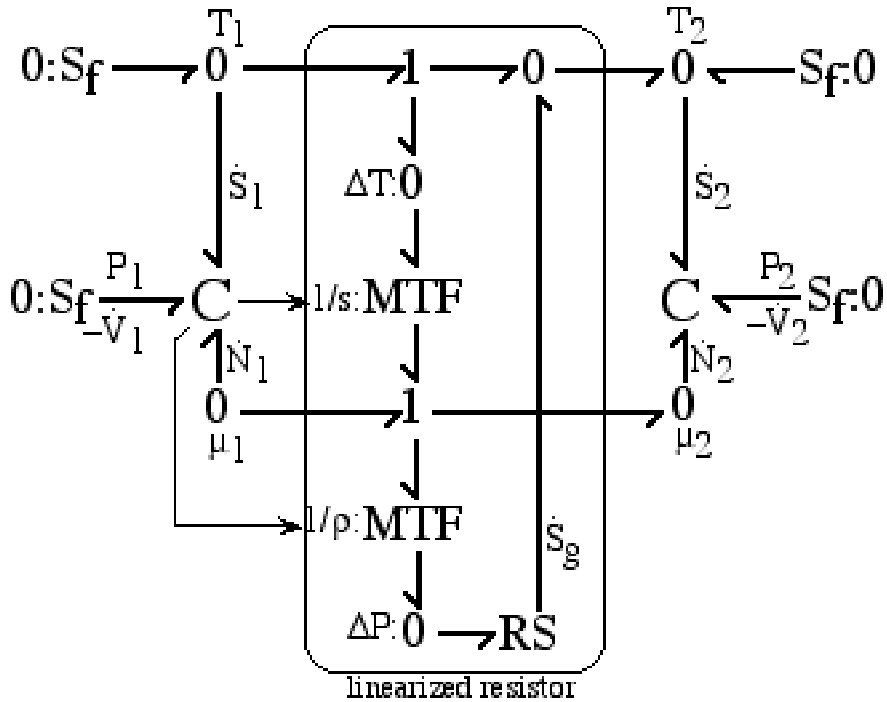
$$\Delta P \approx \frac{\Delta\mu + s\Delta T}{v}$$

or

$$\Delta P \approx \rho(\Delta\mu + s\Delta T)$$

This is a “discretized” version of the Gibbs-Duhem equation

This may be represented by a junction structure
—note the modulated transformers



the modulating factors, specific entropy and specific volume (or density) are taken from the upstream side

the entropy generated is added into the downstream side

(similar to the RS representation of the two-port heat transfer resistor)

NOTE:

$\Delta P \approx \rho_u(\mu_u - \mu_d + s_u(T_u - T_d))$

$\Delta P \approx \rho_u(\mu_u + s_u T_u) - \rho_u(\mu_d + s_u T_d)$

thus

$\mu_u + s_u T_u = h_u$

but

$\mu_d + s_u T_d \neq h_d$

Pressure is NOT computed as a difference of enthalpies

(nor should it be)

Check power flows:

$P_{net,u} = \mu_u dN/dt + T_u s_u dN/dt = h_u dN/dt$

$P_{net,d} = \mu_d dN/dt + T_d s_u dN/dt \neq h_d dN/dt$

in this model, downstream power flow is NOT enthalpy times mass flow

CAUTION:

this junction structure is only valid for small ΔP, ΔT and Δμ

i.e., near equilibrium

COMMENTS:

Despite appearances, enthalpy is not an appropriate effort for mass flow

—it only appears to be because of the coupling between mass and entropy flows

As with all our models, the system is partitioned into equilibrium energy storage and steady-state dissipation

Capacitor

- **satisfies the first law — conserves energy**
- **constitutive equation defined at equilibrium**
- **port displacements are total extensive variables**

Resistor

- **satisfies the second law — generates entropy**
- **constitutive equation defined in steady state**
- **constitutive equations may involve specific variables**

CAUSAL PREFERENCE

This model of throttling is crude

- **Better models may be developed within the same structure**

For modest ratios of upstream to downstream pressures

- **flow velocity exceeds speed of sound**
- **flow becomes “choked”**
- **further decrease of downstream pressure ratio does not increase flow rate**

Models of throttling have a strong causal preference for effort inputs and flow rate outputs

BETTER MODELS OF THROTTLING.

SUBSONIC:

$$dN/dt = C_d A_t \sqrt{\frac{2\gamma}{\gamma-1}\rho_u P_u \left(\left(\frac{P_u}{\rho_u}\right)^{2/\gamma} - \left(\frac{P_d}{\rho_d}\right)^{(\gamma+1)/\gamma}\right)}$$

C_d: discharge coefficient, typically ≈ 0.5

SUPERSONIC:

isentropic flow chokes if $\frac{P_u}{P_d} \geq 0.528$

real gas with flow friction or heat addition chokes sooner

choked flow depends only on upstream pressure

SUPERSONIC CHOKED FLOW:

$$dN/dt = C_d A_t \left(\frac{2}{\gamma+1}\right)^{1/(\gamma-1)} \sqrt{\frac{2\gamma}{\gamma+1}\rho_u P_u}$$

source:

Handbook of Hydraulic Resistance, 3rd Edition, I.E. Idelchik, 1994.