

# Bond Graph Modeling and Simulation of Thermodynamic Systems

For Plenary session, 2007 ICBGM

Forbes T. Brown

Lehigh University, emeritus, Bethlehem, PA

Present address: 1983 Sunderland Drive, Bethlehem, PA 18015

ftb0@lehigh.edu

# Expectations:

- Conventional bond graphs were designed to address systems with “free energy” (mechanical, electrical, magnetic, incompressible fluid) in which all elements are conservative except the Resistance, in which energy is “dissipated” (ceases to be bookkept).
- Thermodynamics also deals with energy, but is more comprehensive in that it includes the thermal form which is not free energy.
- If bond graphs are to become truly widespread, they must accommodate all energies (that is, thermodynamics).
- Because of the innovation of thermal energy, effective bond graphs that represent thermodynamic effects should be expected to involve nonconventional elements.
- In the First Law of Thermodynamics, energy is not dissipated, it is converted to thermal form. Resistance elements do not apply (except in the pseudo bond graph for heat conduction, which is not a true energy-based bond graph).
- The Second Law of Thermodynamics says that thermal energy is only partly convertible to free energy .
- A practical bond graph scheme for thermodynamics requires the efficient calculation of several thermodynamic properties.

# Preliminaries:

- This presentation is downloadable from the Internet; no need to take notes.
- Details not presented are available; see references at end. The coding for most of the simulation examples also is downloadable from the internet.
- Selected references to other authors' approaches are given at the end, with brief comment.
- The author uses the symbol  $T$  rather than  $TF$  for transformer, and  $G$  rather than  $GY$  for gyrator.
- The symbol  $T$  also does double-duty as the modulus of the transformer, defined as the output flow over the input flow.
- Similarly,  $G$  is also the modulus for the gyrator, defined as the ratio of either effort to the opposite flow.

# PART I: NO MASS TRANSFER

Bond graph flow for heat conduction:

Heat conduction:  $\frac{\Theta \text{ (temperature)}}{?}$

Product:  $\dot{Q} = \theta \cdot ?$  (heat flux)

The changed entropy,  $dS$ , of a closed system due to a reversible transfer of heat,  $dQ$ , is defined as  $dS = \frac{dQ}{\theta}$ ,

so that

$$\frac{dS}{dt} = \frac{1}{\theta} \frac{dQ}{dt}$$

or

$$\dot{S} = \frac{1}{\theta} \dot{Q}.$$

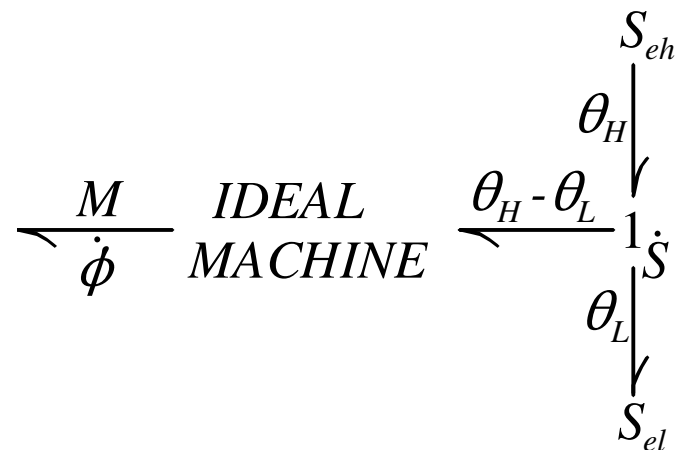
Therefore,

$$? = \frac{\dot{Q}}{\theta} = \dot{S}$$

# Conversion of thermal to free energy:

The entropy,  $S$ , of a closed system cannot decrease, according to the Second Law. A process is **reversible** if  $\dot{S}_{system} = 0$ .

Reversible conversion between thermal and free energy :



Thermal efficiency:  $\eta = \frac{\text{Mechanical work out}}{\text{Thermal power in}}$

$$= \frac{M\dot{\phi}}{\theta_H\dot{S}} = \frac{(\theta_H - \theta_L)\dot{S}}{\theta_H\dot{S}} = 1 - \frac{\theta_L}{\theta_H} \quad (\text{Carnot efficiency})$$

# Entropy production in heat transfer:

Energy conservative couplers:  $e_1 \dot{q}_1 = e_2 \dot{q}_2$

$$\frac{e_1}{\dot{q}_1} \xrightarrow{T} \frac{e_2}{\dot{q}_2} \quad \frac{e_1}{\dot{q}_1} \xrightarrow{G} \frac{e_2}{\dot{q}_2} \quad \frac{e_1}{\dot{q}_1} \xrightarrow{RS} \frac{e_2}{\dot{q}_2}$$

But, by definition,  $\xrightarrow{T}$  and  $\xrightarrow{G}$  are also *reversible*.

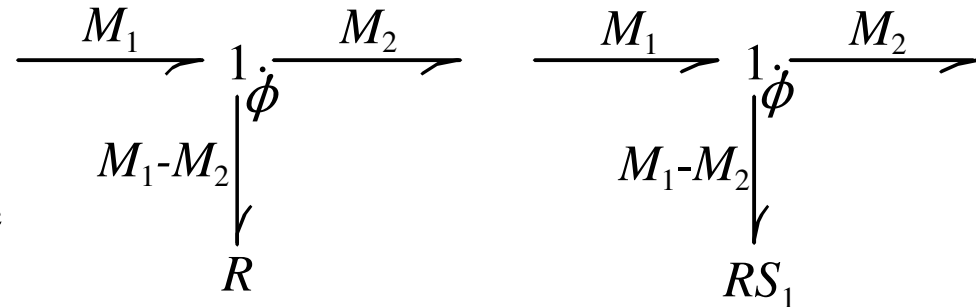
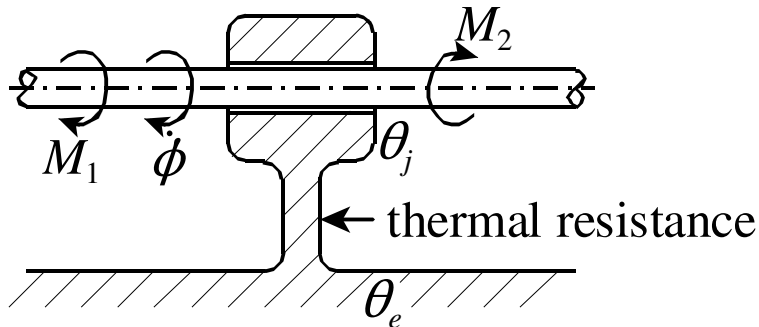
$\xrightarrow{RS}$  is *irreversible*:  $\frac{\theta_1}{\dot{S}_1} \xrightarrow{RS} \frac{\theta_2}{\dot{S}_2}$

Entropy production:  $\dot{S}_2 - \dot{S}_1 = \frac{\theta_1 - \theta_2}{\theta_2} \dot{S}_1$

If, for example, the heat flux is proportional to the temperature difference,  $\dot{Q} \equiv \theta_1 \dot{S}_1 \equiv \theta_2 \dot{S}_2 = H(\theta_1 - \theta_2)$ ,

then  $\dot{S}_2 - \dot{S}_1 = \frac{H(\theta_1 - \theta_2)^2}{\theta_1 \theta_2}$ , which is non-negative regardless of the sign of  $\theta_1 - \theta_2$ .

# Bearing friction – conventional and thermal bond graphs



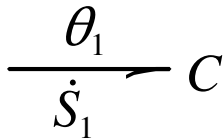
Above: conventional

Opposite: thermal included

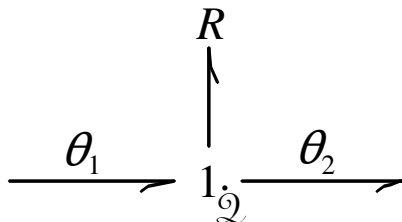
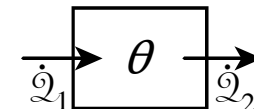
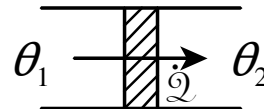
Both graphs can represent the same mechanical behavior, but the thermal graph shows the conversion of mechanical power to thermal form (in  $RS_1$ ) and the temperature drop through the thermal "resistance" (in  $RS_2$ ). Both of these elements represent irreversible processes.

# Thermal compliance:

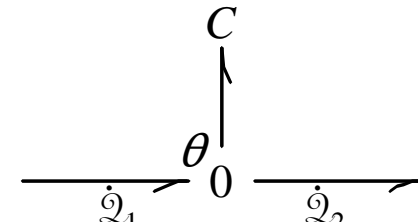
Bond graph:



Pseudo bond graph:



(a) heat conduction

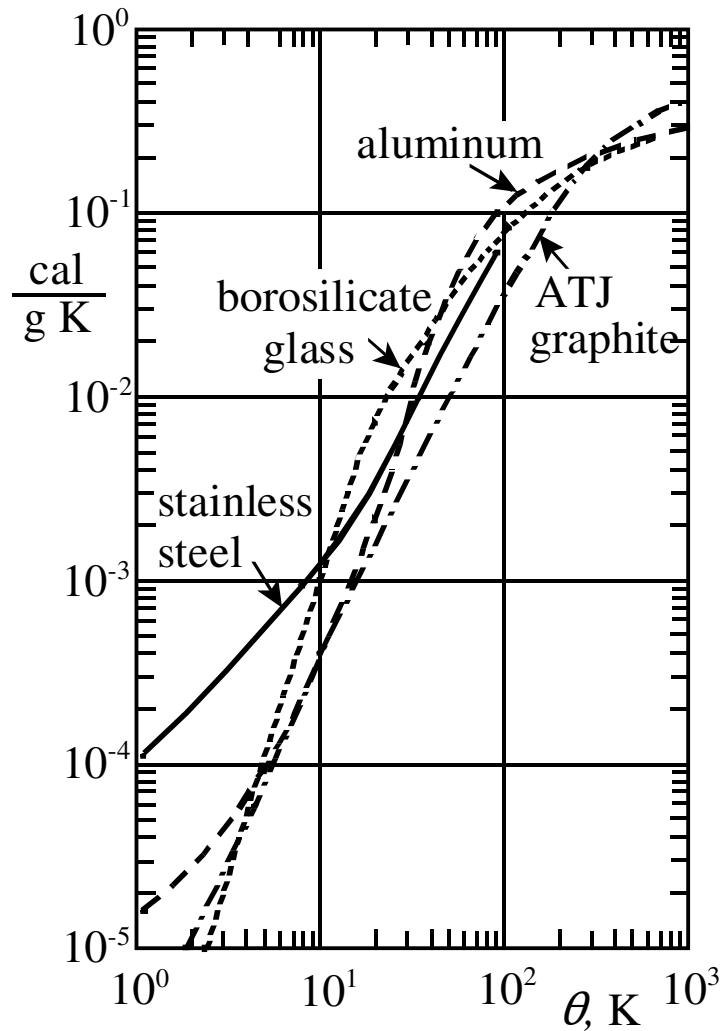


(b) thermal storage

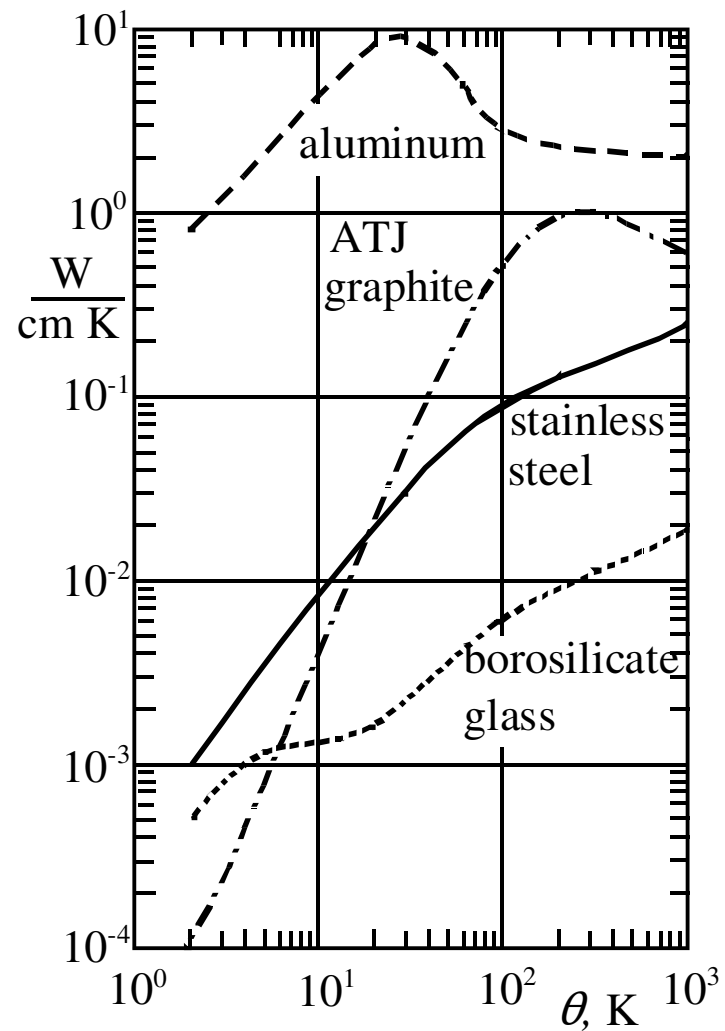
The pseudo bond graph has the advantage of linear relations between its effort and displacement or flow when the specific heat and the thermal conductivity are constant.

But, it is not a true bond graph (the product of its effort and flow is not the energy flux) and therefore it is not compatible with other bond graph elements without *ad hoc* couplings, and . . .

in real life specific heats and thermal conductivities tend not to be constant:

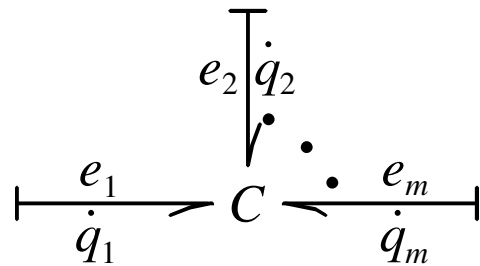


(a) specific heat



(b) thermal conductivity

# The multiport compliance element:



This element, widely used for non-thermodynamic models, also has application for thermodynamic models.

Its potential energy for the integral causality shown is

$$\mathcal{V} = \mathcal{V}(q_1, q_2, \dots, q_m).$$

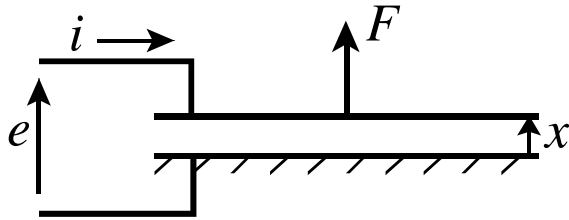
The net input power or energy flux is

$$\mathcal{P} = \sum_{i=1}^m e_i \dot{q}_i = \frac{d\mathcal{V}}{dt} = \sum_{i=1}^m \frac{\partial \mathcal{V}}{\partial q_i} \frac{dq_i}{dt}.$$

Since this result applies regardless of the magnitudes of the individual  $\dot{q}_i$ , the key result is the theorem of virtual work::

$$e_i = \frac{\partial \mathcal{V}}{\partial q_i}, \quad i = 1, 2, \dots, m.$$

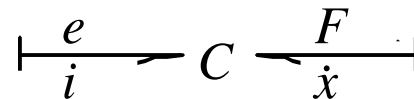
# Non-thermodynamic example: a variable plate capacitor



Neglecting fringing, the capacitance is

$$C = \frac{\epsilon A}{x}, \quad \text{where } A \text{ is area and } \epsilon \text{ is the dielectric constant.}$$

The bond graph is



Electrostatic energy:

$$\mathcal{V} = \frac{1}{2C} q^2$$

Voltage,  $e$ , and force,  $F$ :

$$e = \frac{\partial \mathcal{V}}{\partial q} = \frac{q}{C} = \frac{xq}{A\epsilon}$$

$$F = \frac{\partial \mathcal{V}}{\partial x} = \frac{q^2}{2\epsilon A} = \frac{\epsilon A e^2}{2x^2}$$



# Lead-acid battery, differential causality problem

To generate the equations for nonlinear compliance or inertance elements a Legendre transformation may be made. Since these 2-port compliances have differential causality only on their thermal sides, Esperilla et al made the Legendre transformations of the energies in these elements with respect to the thermal ports only:

$$G \equiv \mathcal{L}(\mathcal{V}) = \mathcal{V} - \theta S,$$

or, since  $d\mathcal{V} = e dq + \theta dS$ ,

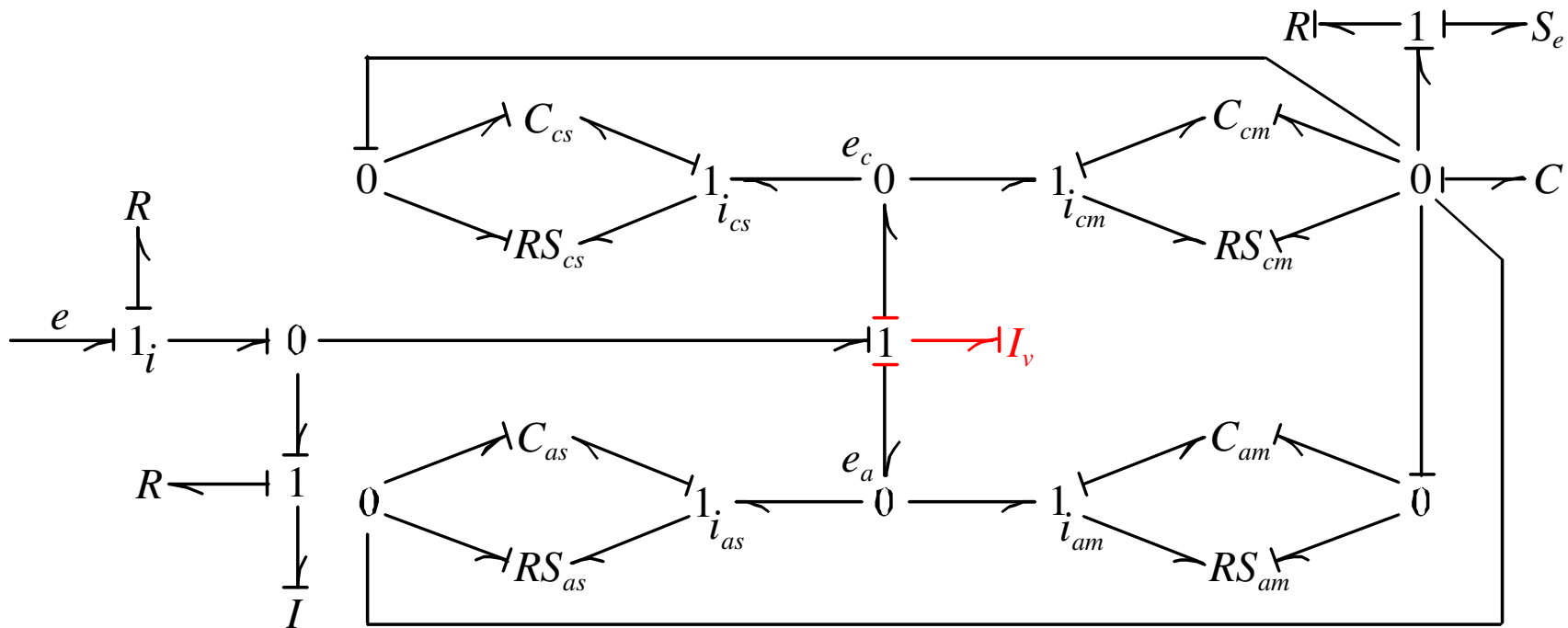
$$dG = e dq - S d\theta.$$

$G$  is treated as a state function, giving the differential causality result

$$\dot{S} \equiv \frac{d}{dt}(S); \quad S = -\frac{\partial G}{\partial \theta}.$$

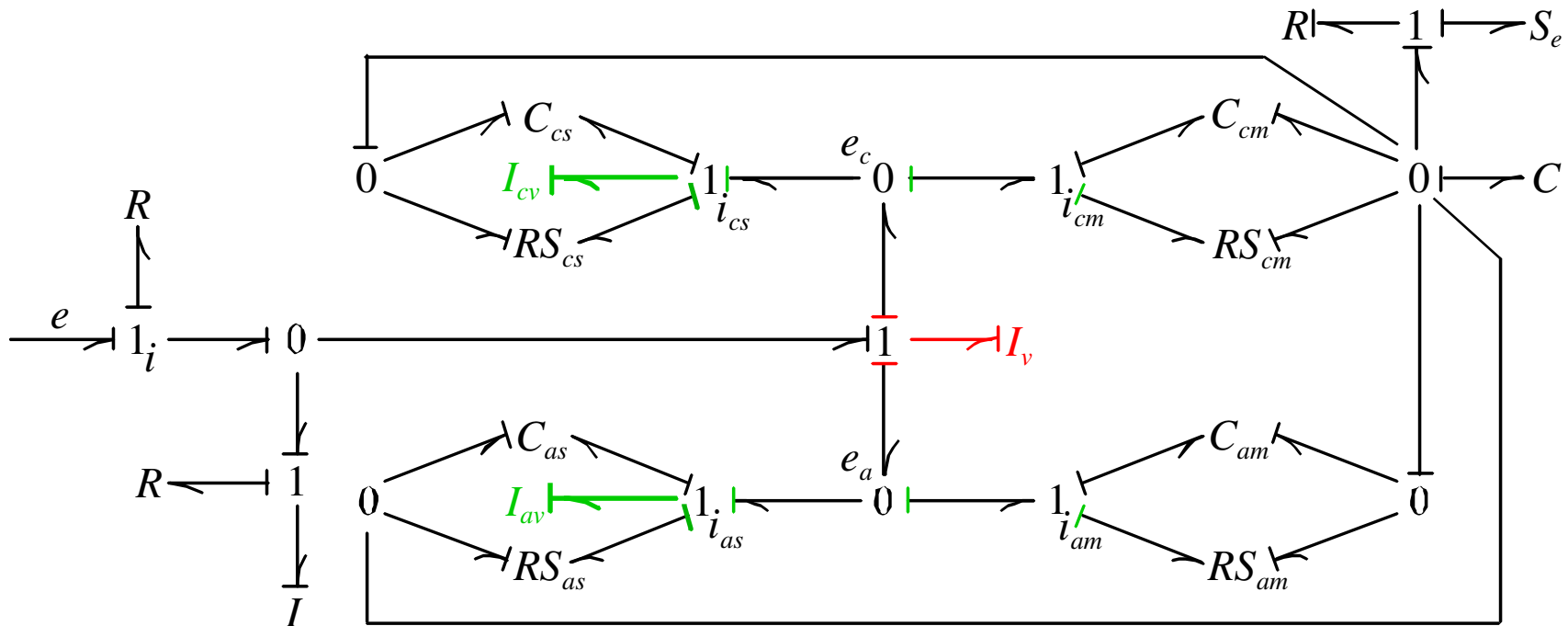
# Lead-acid battery, undercausality problem:

Undercausality (not all bonds having mandated causality) for any bond graph implies that one or more algebraic equations are needed, in addition to the differential equations, to form a DAE system of equations. To get the algebraic equations, one can apply a virtual inertance to a 1-junction with incomplete causality or a virtual compliance to a 0-junction with incomplete causality:



# Undercausality, continued:

The virtual inertance in red does not force all of the causal strokes; two more virtual inertances, shown in green, are needed:



Setting the efforts on the three virtual inertances to zero generates three algebraic equations. Esperilla *et al* chose instead to set very small values for these inertances, in order to substitute differential equations. There is a compromise between accuracy and the computational stiffness of the resulting set of differential equations.

# PART II: MASS TRANSFER

## The convection bond

The rate of energy transfer in an assumed uniform stream of a pure substance with pressure  $P$ , mass density  $\rho$ , internal energy  $u$ , velocity  $v$  and mass flow  $dm/dt$ , omitting gravity effects, is

$$\dot{\mathcal{P}} = \left( \frac{P}{\rho} + u + \frac{v^2}{2} \right) \dot{m},$$

The sum of the first two terms in parenthesis is defined as the **enthalpy**,  $h$ , and the sum of all three is the **stagnation enthalpy**,  $h_0$ , suggesting the effort and flow  $\frac{h_0}{\dot{m}}$

Omitting for the moment the velocity, the problem with this representation is that the enthalpy does not describe the state of the substance; the state postulate says that *two* independent variables are needed.

# The convection bond, continued

Thus, although there is a single flow, two effort variables are needed to describe the situation. There is considerable choice regarding which two to use. One possibility uses the (Gibbs) free energy effort,  $g$ , and the thermal effort  $\theta s$ . For most purposes, however, it seems best to use the enthalpy,  $h$ , (omitting velocity effects) and the pressure,  $P$ :

$$\frac{P, h}{\dot{m}} \rightarrow$$

The pair of lines that comprise the bond suggest the presence of the two effort variables. Note that the actual effort is  $h$ , and  $P$  is the qualifier. The direction half-arrow designates which way represents positive flow (since  $h$  is never negative). A causal stroke at either end of the bond refers to the causality of  $P$ ;  $h$  is naturally causal in whichever direction the flow is going.

$P$  determined from left:  $\frac{P, h}{\dot{m}} \rightarrow$        $P$  determined from right:  $\leftarrow \frac{P, h}{\dot{m}} \rightarrow$

The flow  $\dot{m}$  is causal in the opposite direction from  $P$ , as with any bond.

# The *RS* element for fluid flow

When applied to convection bonds, the *RS* element describes the effect of a fluid valve or other restriction:

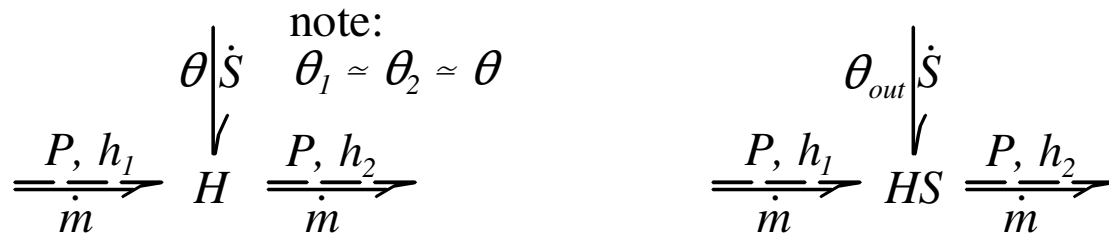
$$\begin{array}{c} P_1, h \\ \hline \dot{m} \end{array} \begin{array}{c} \text{---} \\ | \\ \text{---} \end{array} RS \begin{array}{c} P_2, h \\ \hline \dot{m} \end{array}$$

The mass flow and the enthalpy (or stagnation enthalpy when the velocity is significant), and as a result the energy flux, is the same on both sides of the element, despite the pressure difference. The thermodynamic availability (convertibility of the thermal energy to free forms) is reduced on the downstream side, however, and entropy is created.

The causal strokes shown in red represent the most common of the four possibilities. In this case, the mass flow and whatever other properties are of interest are computed from knowledge of the two pressures and the upstream enthalpy. The standard equations for the choked and unchoked flow of an ideal gas through an orifice, for example, can be placed in this form.

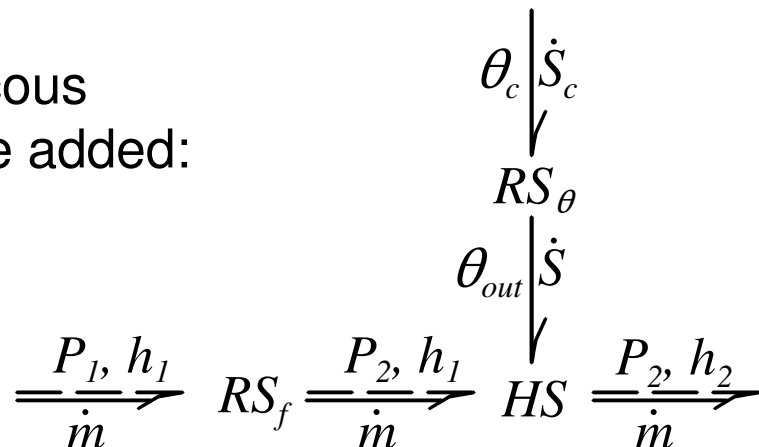
# Heat interaction elements

A special reversible heat interaction element is shown on the left below, and a more general irreversible such element on the right:



Viscosity induced wall shear is omitted, which can be shown makes the input and output pressures equal\*. The  $H$  element applies only when the rate of heat transfer is infinitesimal or the fluid doesn't change temperature because it is in the two-phase region.

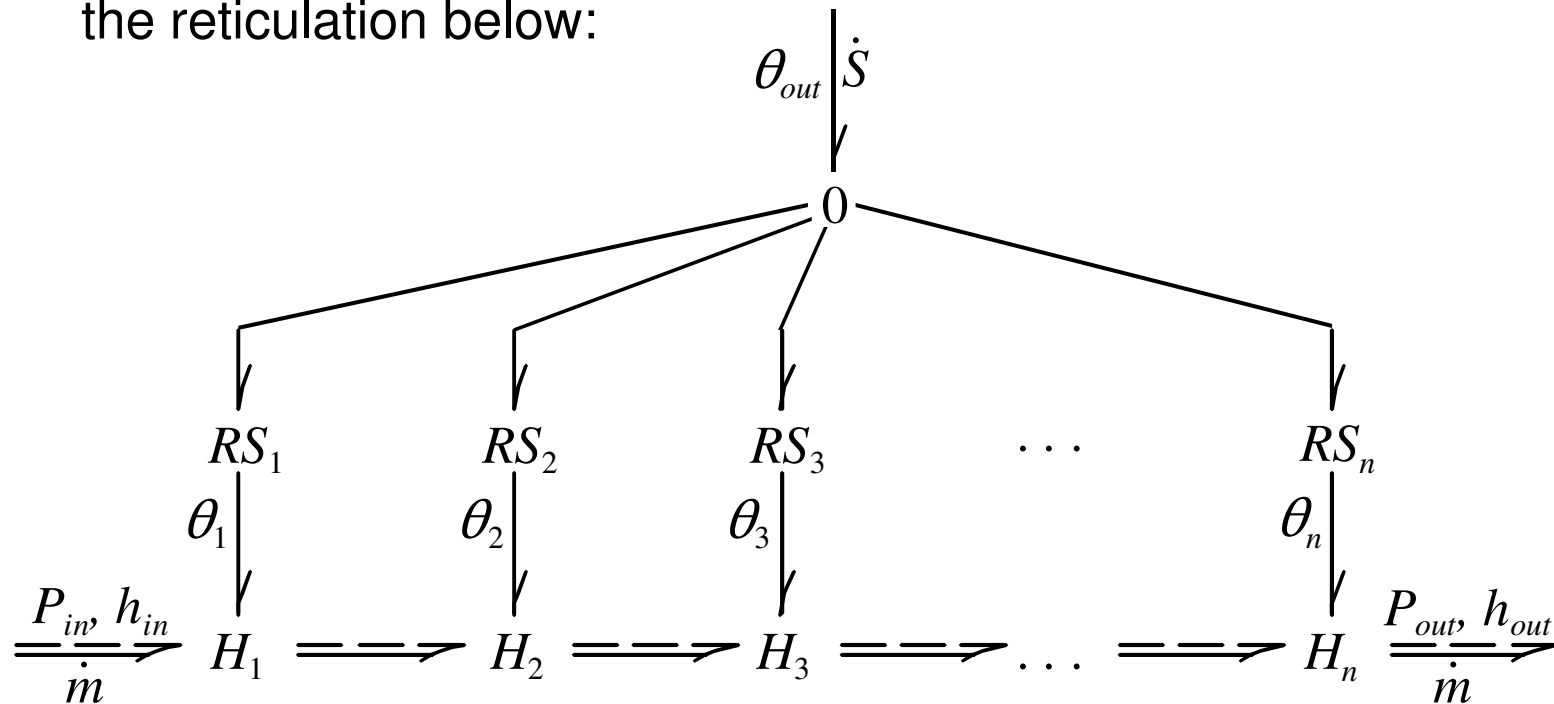
Additional irreversibilities from viscous friction and heat conduction can be added:



\* Heat transfer itself implies some wall shear. Proper treatment requires use of stagnation rather than static temperatures.

# Heat interaction elements, continued

The meaning of the *HS* element can be understood in terms of the reticulation below:



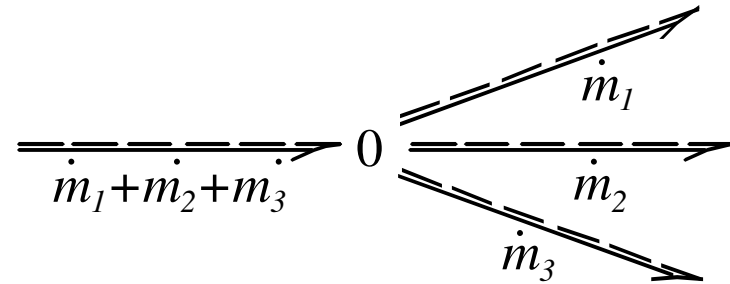
Irreversibility occurs in the *RS* elements.

Assuming the fluid is not in the two-phase region, only the specific heat is necessary to compute  $h_{out}$ :

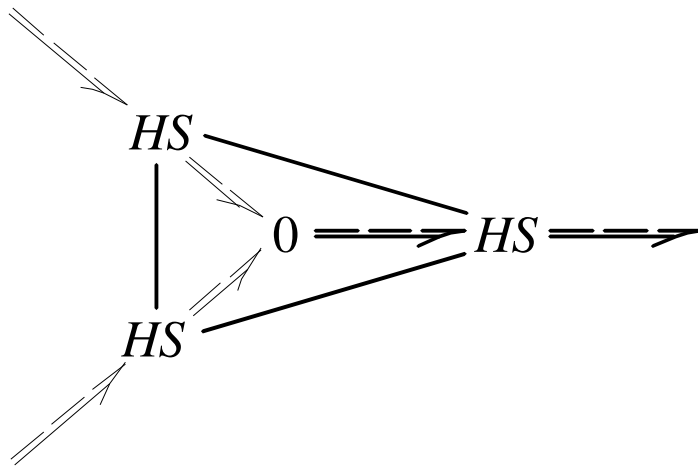
$$h_{out} = h_{in} + \frac{(\dot{S} / \dot{m})\theta_{in}}{1 - \dot{S} / c_p \dot{m}}$$

# The 0-junction for convection bonds

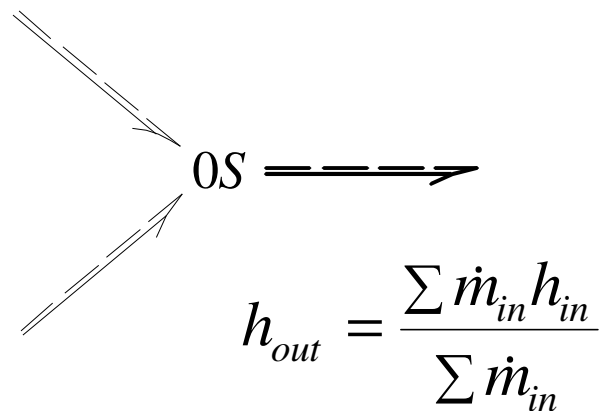
Use of a standard 0-junction with convection bonds makes sense only if *both* of the effort variables (e.g.  $h$  and  $P$ ) are common. This applies to diverging flows at a junction:



For general merging flows that have different temperatures (but a common pressure) the needed combination is:



In practice this is replaced by the 0S junction below, which is implemented by the simple computation given:

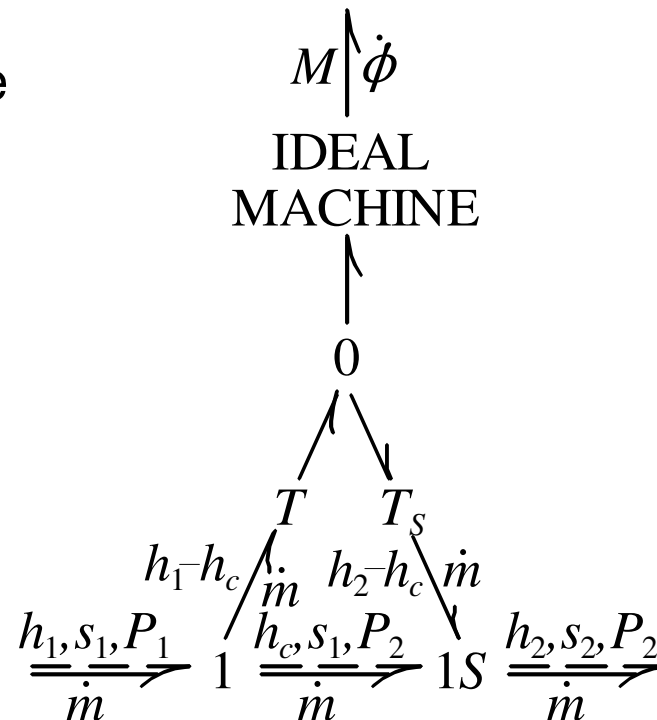


# The 1- and 1S-junctions with convection

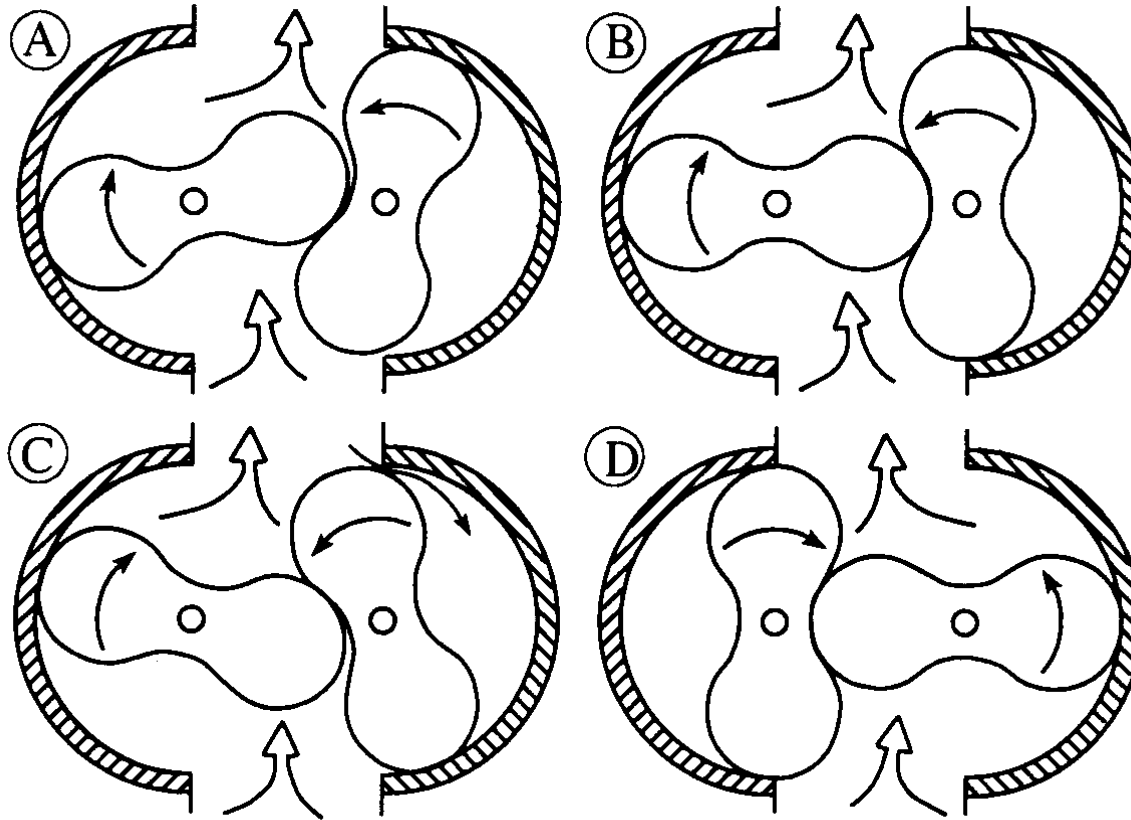
1-junctions conserve energy, are irreversible and have common flow on all bonds; since there is only one flow, that meaning is unambiguous, unlike 0-junctions. The entropies on the input and output convection bonds must be equal. It also is helpful to define an energy-conservative but irreversible 1S-junction in which the *pressures* on the input and output convection bonds are equal.

Both types are used in the example of an adiabatic fluid machine that suffers losses due to friction and/or internal leakages, characterized by its volumetric efficiency,  $\eta_v$ , and its adiabatic efficiency,  $\eta_{ad}$ . It can be shown that

$$T = \frac{\eta_v}{\eta_{ad}}; \quad T_S = \frac{1}{\eta_v(1/\eta_{ad} - 1)}.$$



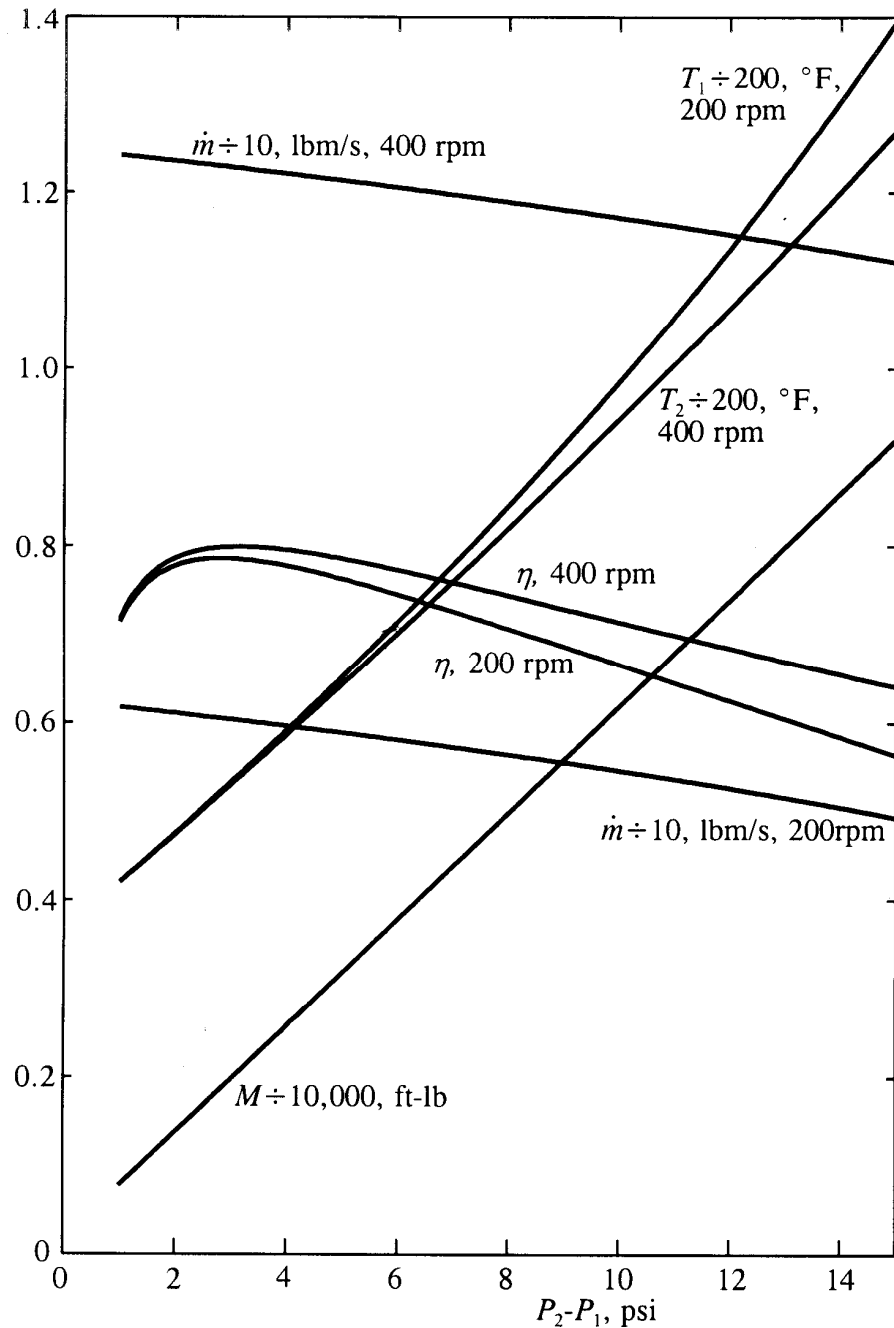
# Example of two-impeller straight-lobe rotary compressor (Roots blower)





# Roots blower - results

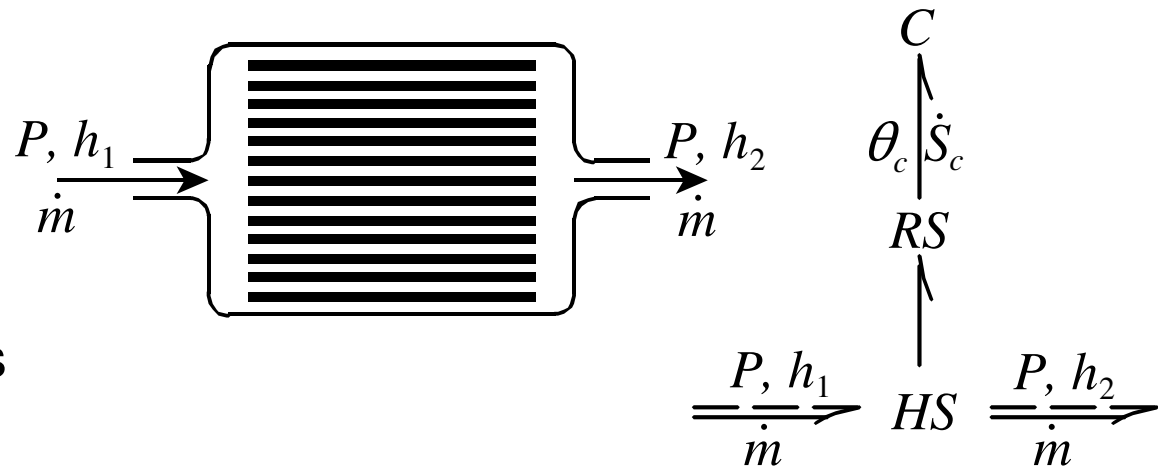
These results agree well with data. Some parameters were chosen to effect this match. The entropy produced in the various elements can be computed, potentially aiding the design.



# Convection elements and compliance

The major interest in using bond graphs is to model and analyze dynamic systems, which implies the use of energy storage elements. Thermodynamic energy is represented by compliance elements, and generally is much larger than coherent kinetic energy, which is addressed later. Dynamic models often are easier to treat computationally than steady-state models, since there are fewer algebraic equations to combine.

The simple-bonded conduction compliance sometimes is combined with convection bonds, as in the case of the thermal regenerator.



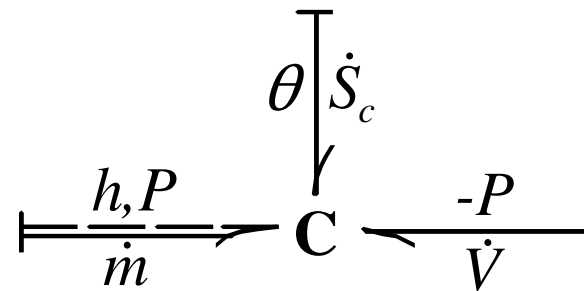
# The general thermodynamic compliance

Consider a system or control volume of volume  $V$  containing a pure substance with mass  $m$  at temperature  $\theta$  and pressure  $P$  representing specific internal energy  $u$ , enthalpy  $h$ , and entropy  $s$ . The rate of change of the total thermodynamic energy of this substance is

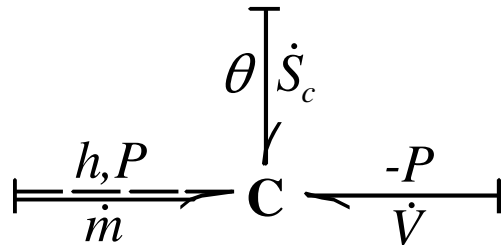
$$\frac{d\mathcal{V}}{dt} = h\dot{m} + \theta\dot{S}_c - P\dot{V}.$$

The first term on the right represents energy transported into the volume by mass flux. The second term represents thermal energy that enters by heat conduction, with entropy flux  $S_c$ . The third term represents pressure work done when the volume itself changes.

This gives a 3-port compliance element with one convection bond for the mass transport and two simple bonds for the heat and work. Note the integral causality.



# Ideal state variables



The causal input variables can be integrated to give  $m$ ,  $V$  and the entropy

$$S = \int (\dot{S}_c + s\dot{m}) dt.$$

In practice it is simplest to deal with the specific properties

$$u = \mathcal{U} / m; \quad \rho = m / V; \quad s = S / m.$$

This suggests the use of  $s$  and  $\rho$  as the thermodynamic state variables, which implies the state equation in the form

$$u = u(s, \rho).$$

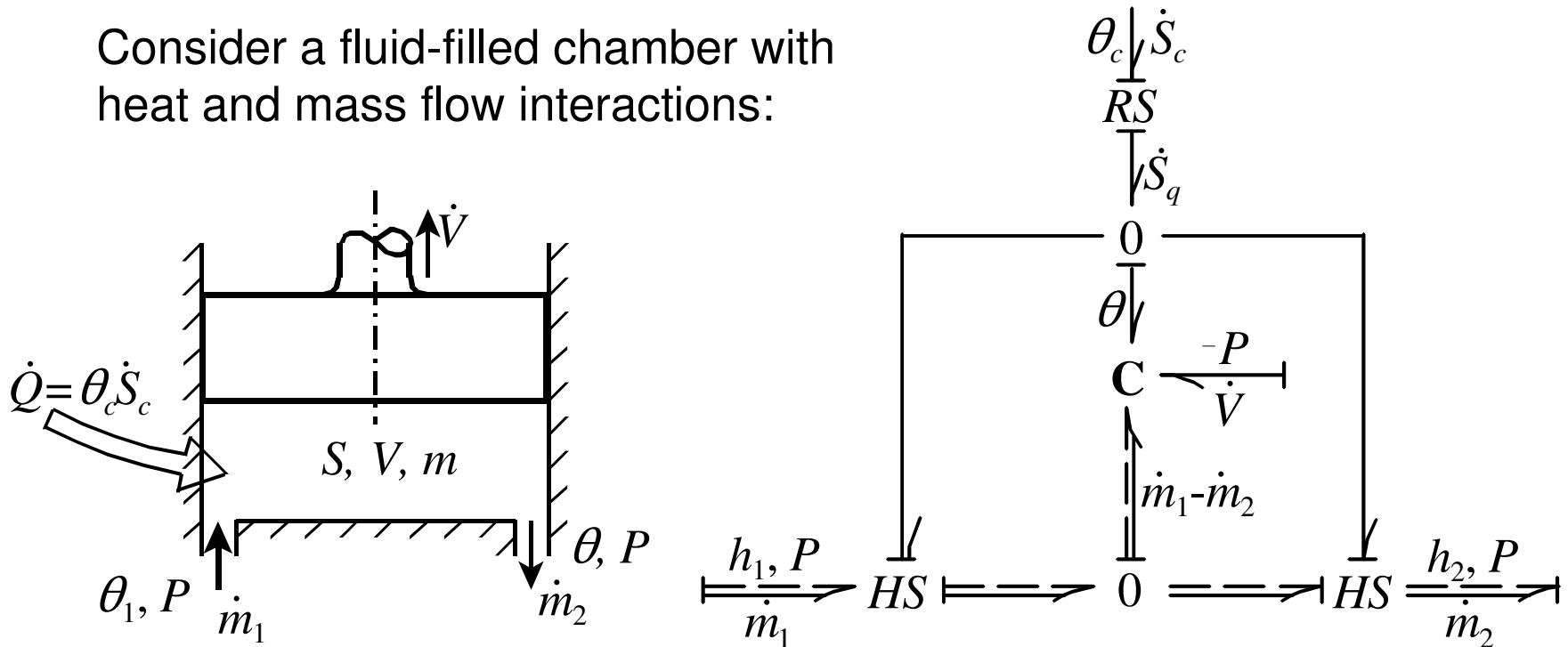
If this state equation is known for the given substance, the output variables can be computed using

$$\theta = \left( \frac{\partial u}{\partial s} \right)_{\rho}; \quad P = \rho^2 \left( \frac{\partial u}{\partial \rho} \right)_s; \quad h = u + \frac{P}{\rho}.$$

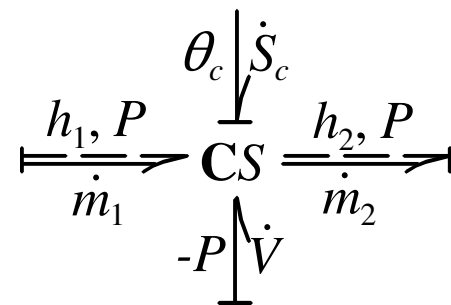
This state equation is not generally known, unfortunately.

# The CS macro element

Consider a fluid-filled chamber with heat and mass flow interactions:



This combination is recognized as the **CS** macro element, the use of which usually precludes the need to use separate  $H$  and  $HS$  elements:



## CS macro element, continued

The properties of pure substances normally are given in the form of “ $P, v, T$ ” equations and specific heat at zero volume equations:

$$P = P(v, \theta); \quad c_v^0 = c_v^0(\theta); \quad v \equiv 1/\rho.$$

Some substances have state equations in terms of the Helmholtz free energy  $\psi = u - \theta s$ :

$$\psi = \psi(v, \theta).$$

Both of these are functions of the temperature,  $\theta$ , and the specific volume,  $v$ , which therefore become the preferred thermodynamic state variables. They lead to the form  $u = u(v, \theta)$ .

The state differential equations for  $dV/dt$  and  $dm/dt$  are determined causally from the external bonds, and it can be shown that the third and final state differential equation is

$$\frac{d\theta}{dt} = \frac{1}{m \partial u / \partial \theta} \left[ \dot{Q} + \sum_i (h_i - h) \dot{m}_i + \left( P + \frac{\partial u}{\partial v} \right) (v \dot{m} - \dot{V}) \right].$$

# CS macro element, continued

Application of this equation in the saturated vapor two-phase region requires some elaboration. It is most convenient to use available or deducible formulas of the following forms, where  $v_g$  stands for saturated vapor:

$$P \equiv P_{sat} = P_{sat}(\theta); \quad v_g = v_g(\theta).$$

The practical result is

$$\frac{d\theta}{dt} = \frac{1}{denom} \left[ \dot{Q} + \theta \frac{dP_{sat}}{d\theta} (v\dot{m} - \dot{V}) + \sum_i (h_i - h)\dot{m}_i \right],$$

$$denom = m \left[ \left( \frac{\partial u_g}{\partial v_g} + P_{sat} - \theta \frac{dP_{sat}}{d\theta} \right) \frac{dv_g}{d\theta} + \frac{\partial u_g}{\partial \theta} - \theta \frac{d^2 P_{sat}}{d\theta^2} (v_g - v) \right].$$

The many derivatives on the right sides of these equations can be determined analytically before evaluation. It would not be practical to label all variables of interest as efforts or flows on a conventional bond graph, supporting the idea of the shorthand convection bond.

# Coding for evaluation of thermodynamic properties

The first reference at the end of this presentation lists coding that calculates 20 dependent properties or derivatives for the refrigerants R12 and R134a, 10 properties or derivatives of water, gaseous air, oxygen and nitrogen, and 4 properties of ideal gas, given two independent variables. This coding is downloadable from the internet, as will be described.

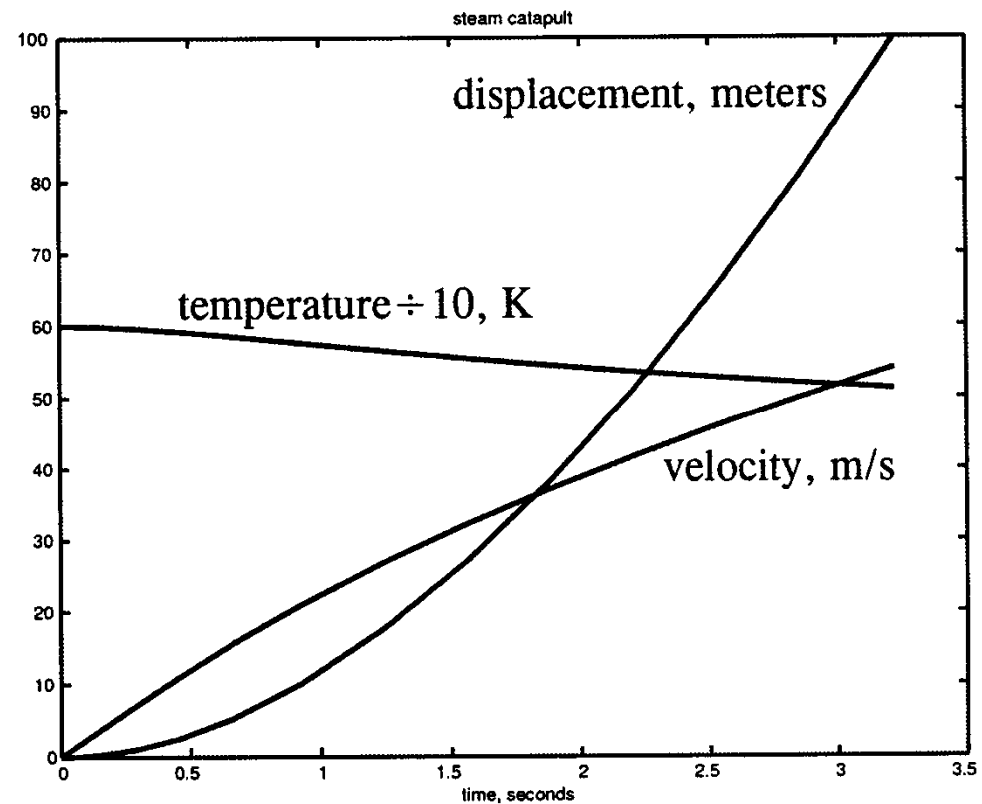
A coding package should become downloadable within the next couple months that will compute 29 properties of interest (16 of which apply only in the saturated mixture region) for probably 13 elements, 12 refrigerants, 9 hydrocarbon fuels and 6 other compounds. The program structures are streamlined to reduce redundancy, increase computational efficiency and allow ready expansion of the list of substances. Iteration is not used. Includes compressed liquid for most substances.

# Case study: steam-driven catapult

Closed chamber, no heat transfer,  
filled with two-phase steam,  
expanding against a piston which  
accelerates an aircraft:

$$C S \frac{P}{\dot{V}} \rightarrow T \frac{\dot{p}}{p/A} \rightarrow I$$

Simulation results:



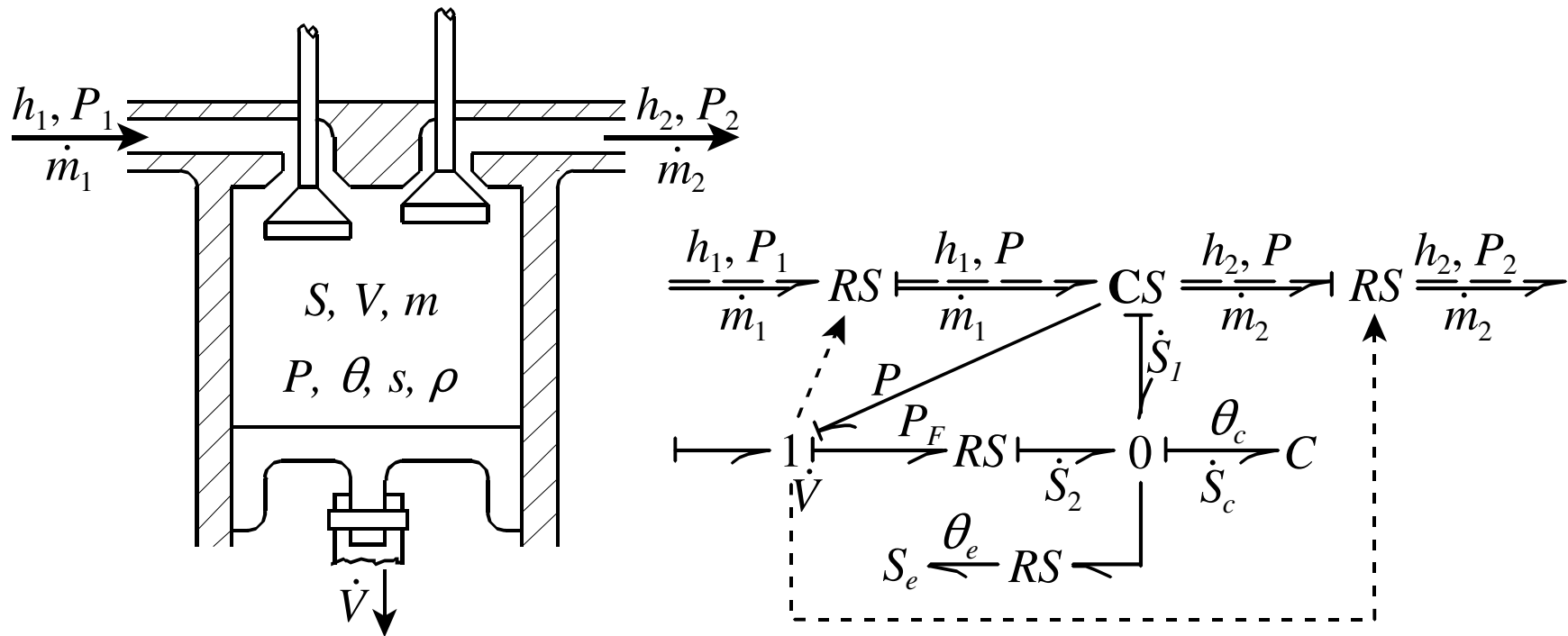
# Steam-driven catapult: MATLAB® coding

```
Global Ac m I F0 V0
V0=.4; Ac=.024; T0=600; v0=.002; m=V0/v0; I=16000; F0=100000;
waterdat
[t,x]=ode45('catpltd',[0 3.22],[T0 0 0]);
plot(t,x(:,3),t,x(:,2)/16000,t,x(:,1)/10)

Function f=catpltd(t,x)
% x(1) is temperature of water/steam; x(2) is aircraft momentum
% x(3) is aircraft position; the eq'n dV/dt=Ac/I*x(2) is in f(1)
Global Ac m I F0 V0
v=(V0+Ac*x(3))/m; T=x(1)
[P,h,vg,dvg,dudT,dudv,dugdT, dugdvg,dPs,d2Ps]=propwat(v,T);
P=P*1e6; dPs=dPs*1e6; d2Ps=d2Ps*1e6;
dugdvg=dugdvg*1000; dugdT=dugdT*1000;
d=m*((dugdvg+P-T*dPs)*dvg+dugdT-m*T*d2Ps*(vg-v));
f(1)=-T*dPs*AC/I*x(2)/d;
f(2)=F0+Ac*P;
f(3)=x(2)/I; f=f';
```

# Case study: a piston-cylinder air compressor

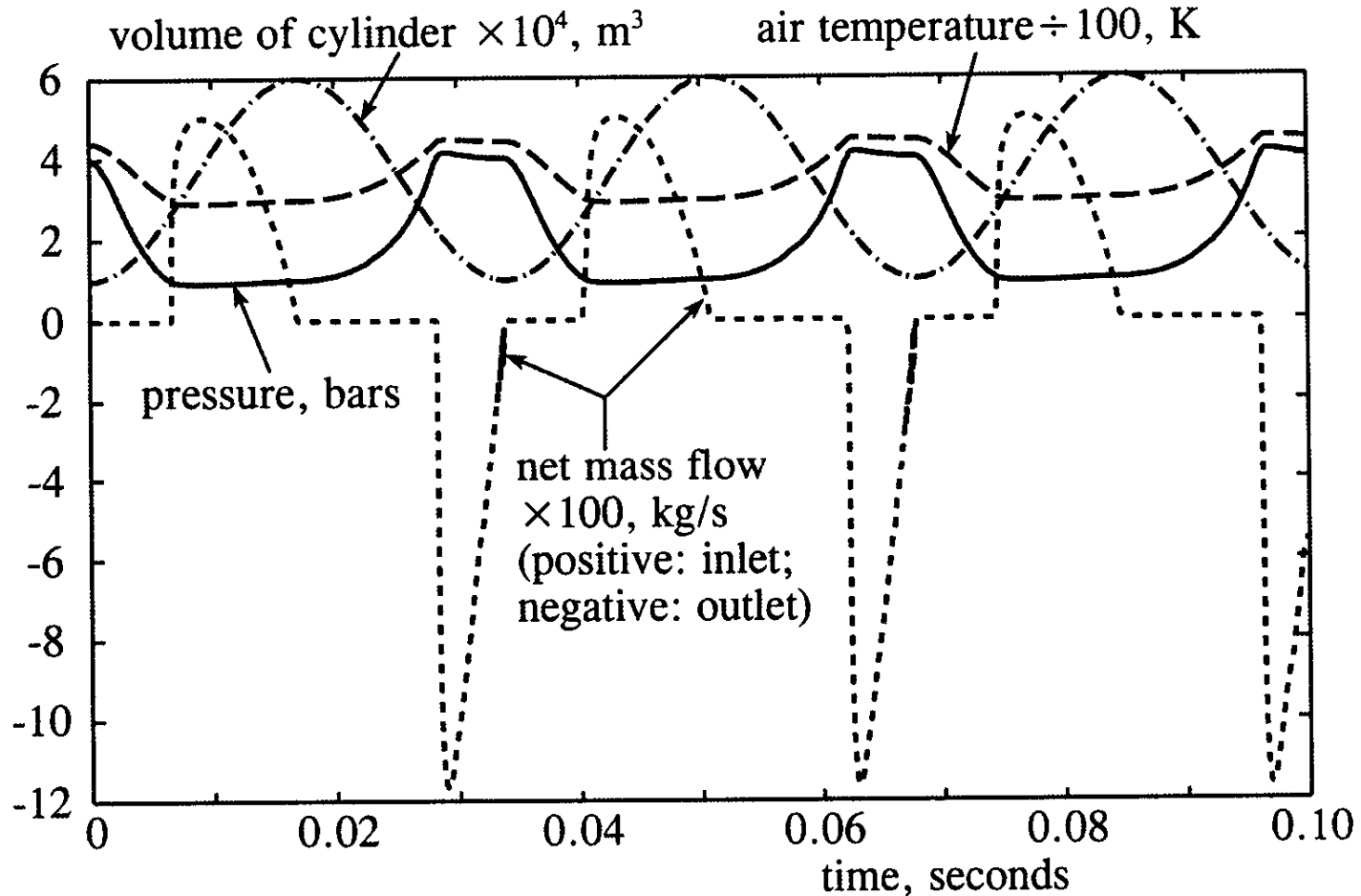
This one-cylinder machine is modeled as below:



The openings of the valves are controlled externally by the direction of motion of the piston, explaining the dashed lines.  $C$  represents thermal energy in the walls, and there is heat conduction to the environment at temperature  $\theta_e$ .

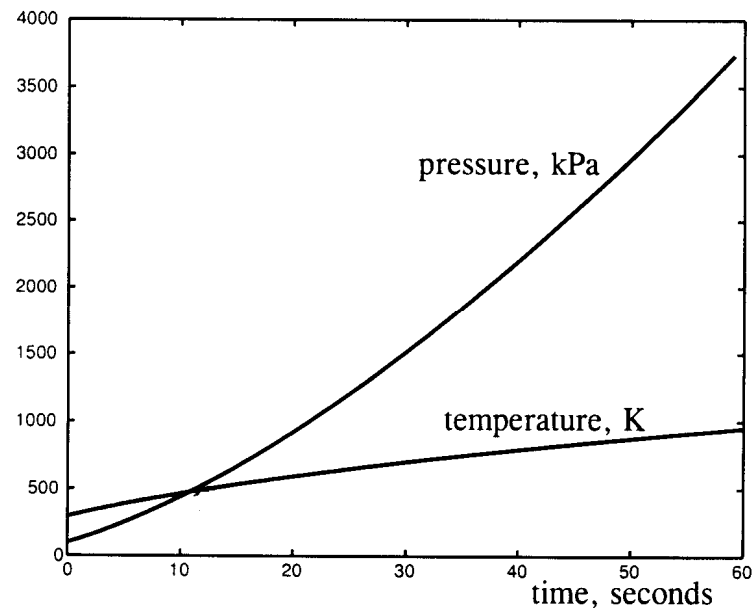
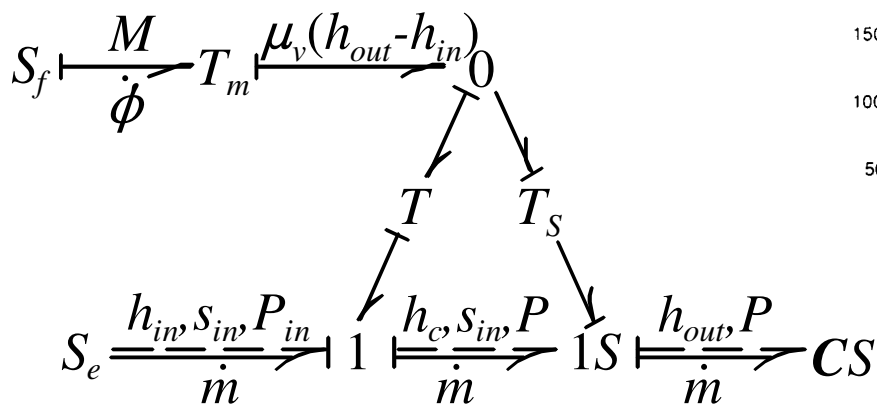
# Piston-cylinder air compressor: simulation results

Simulation results with the assumption of the valves either being at a fixed open position or closed, with flow calculated from an ideal gas orifice equation, are



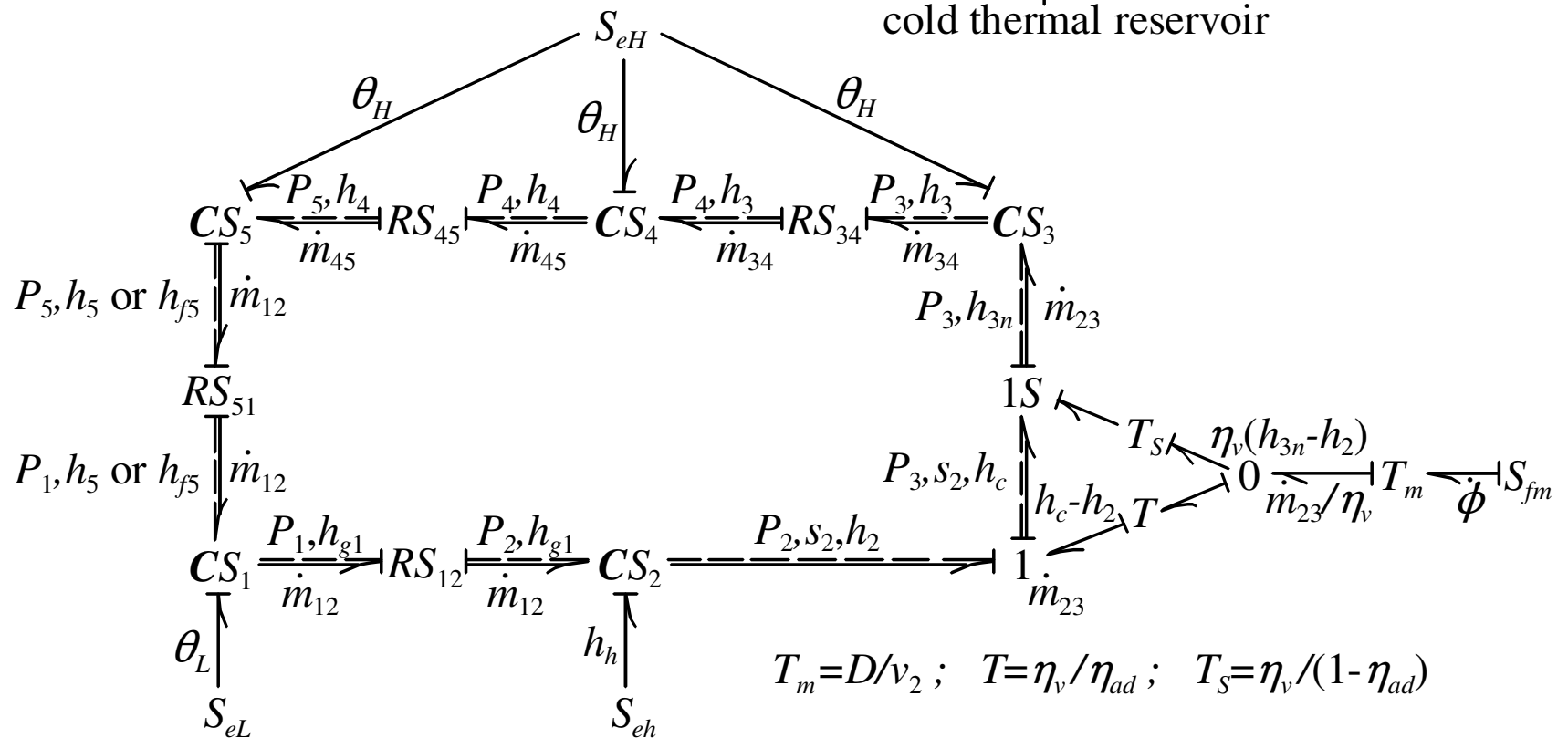
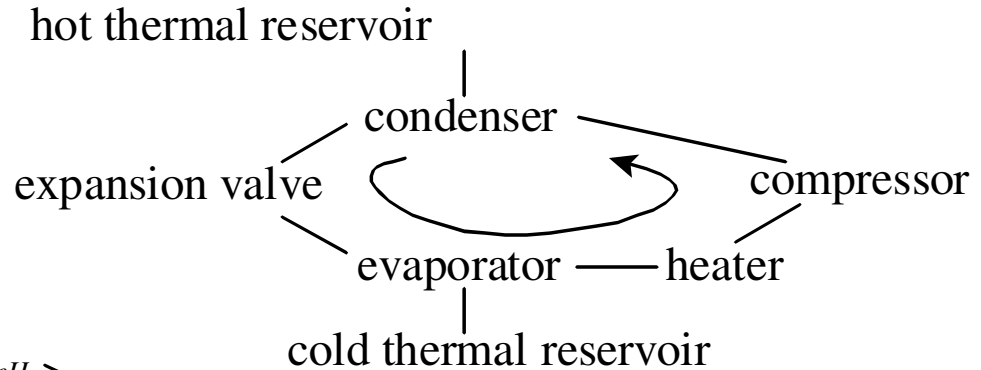
# Piston-cylinder air compressor charging tank

There may be little interest in the details of each cycle if a process requires dozens or hundreds of cycles. The compressor is approximated below, as earlier, by a quasi-steady model with known adiabatic efficiency (80%) and volumetric efficiency (95%). It is charging a tank. Each cycle takes about two seconds.



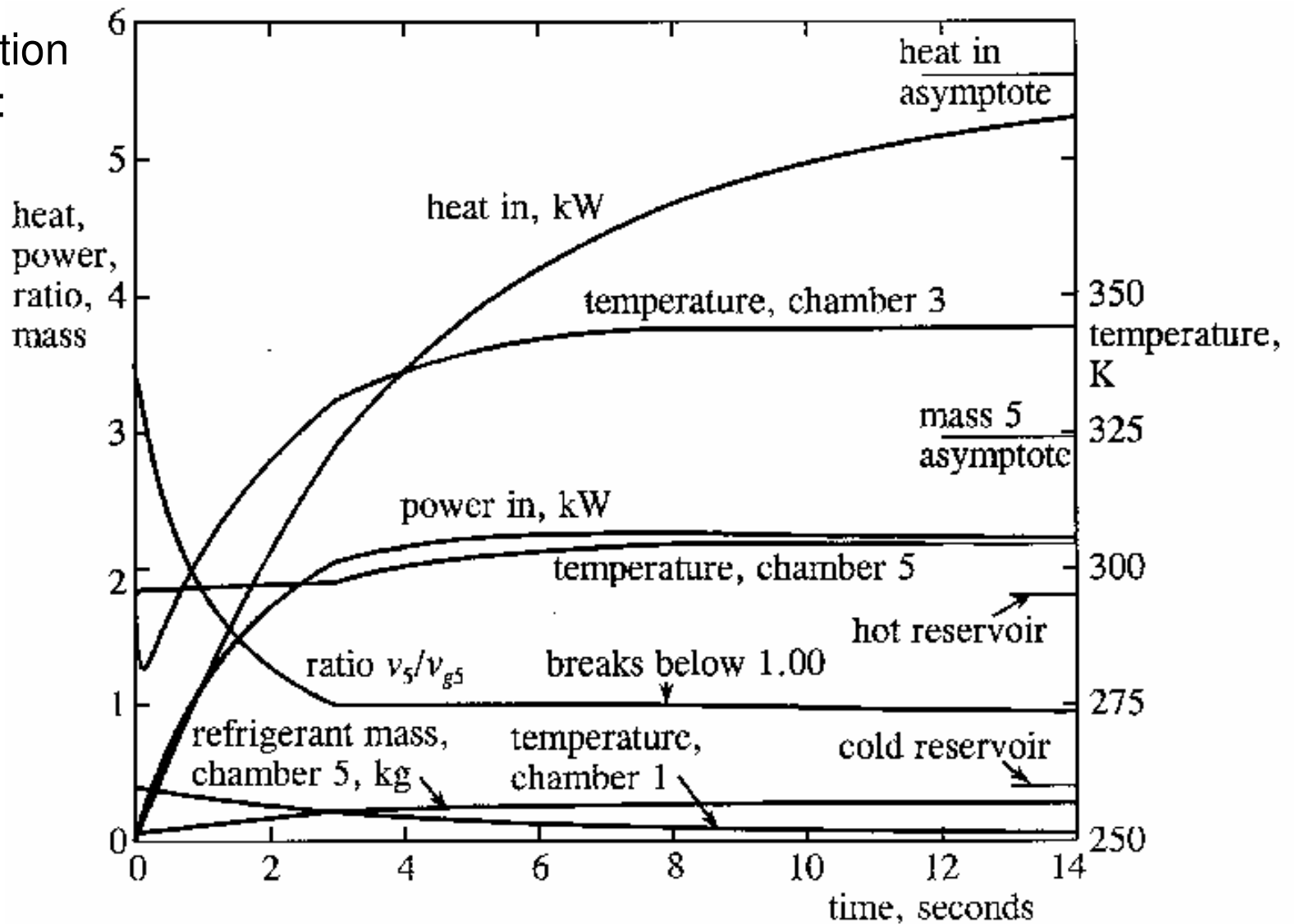
# Start-up of a refrigerator

The schematic of a refrigeration cycle opposite is modeled crudely below.



# Start-up of a refrigerator, continued

Simulation results:



# Fluid inertance in compressible flow

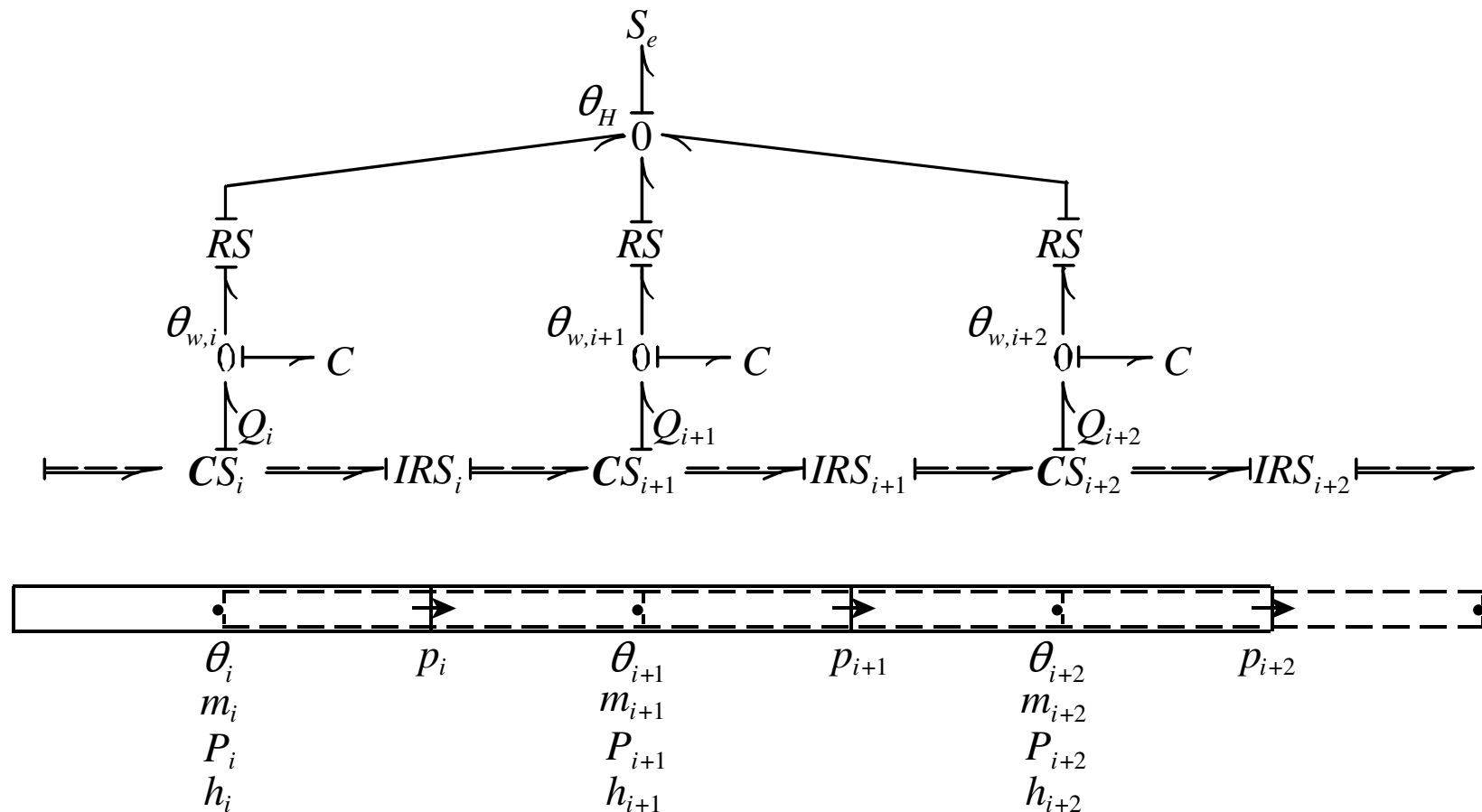
The *incoherent* kinetic energy of fluid molecules has been included in the fluid compliance. The *coherent* kinetic energy of a fluid is represented in an inertance. The use of proper inertance elements permits direct dealing with actual as opposed to stagnation properties.

Combining inertial and resistance effects into a single element, called the *IRS* element, is recommended. This combination effectively represents the momentum balance of the flow to which it applies.

The combination of fluid compliance and inertance, for example in a long tube, produces wave effects. Although inertance effects are often small enough to be neglected, they can be accommodated by alternating several lumped compliance and inertance elements, as in non-thermodynamic cases. These elements best represent overlapping and staggered control volumes, which lead automatically to what is known in the non-bond graph literature as the standard method of *staggered grids*.

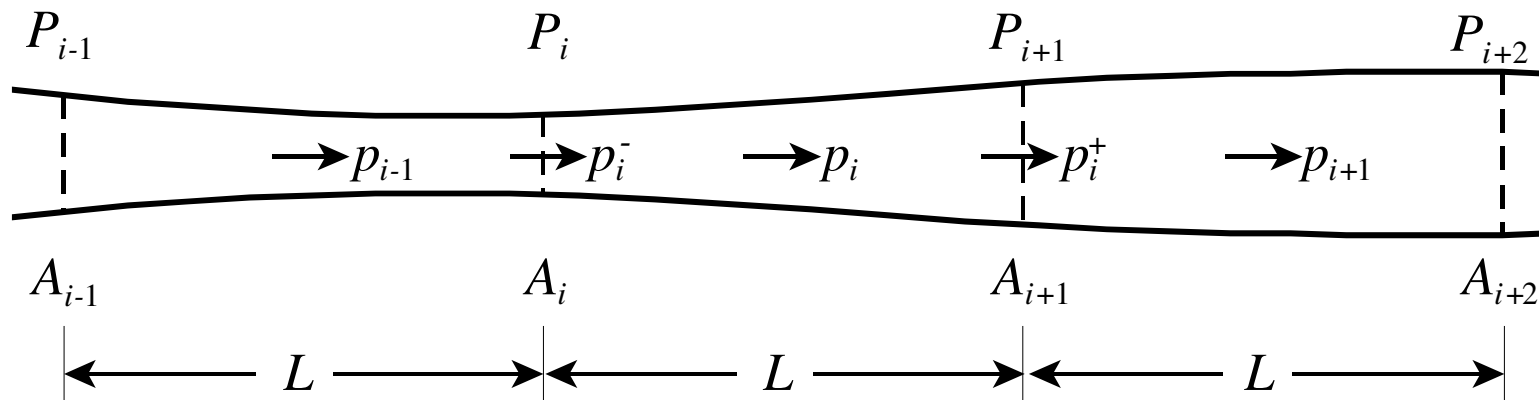
# Fluid inertance in compressible flow, continued

A segment of a channel containing possibly a two-phase mixture some places and a vapor or a liquid in other places (such as the condenser in a refrigeration system) is modeled below. Heat is transferred to the walls and from there to the environment.



# Fluid inertance in compressible flow, continued

Control volumes for the IRS elements are shown below, allowing changes in the area of the channel. The wall shear force  $F_{w,i}$  depends on the local liquid and vapor Reynolds numbers.



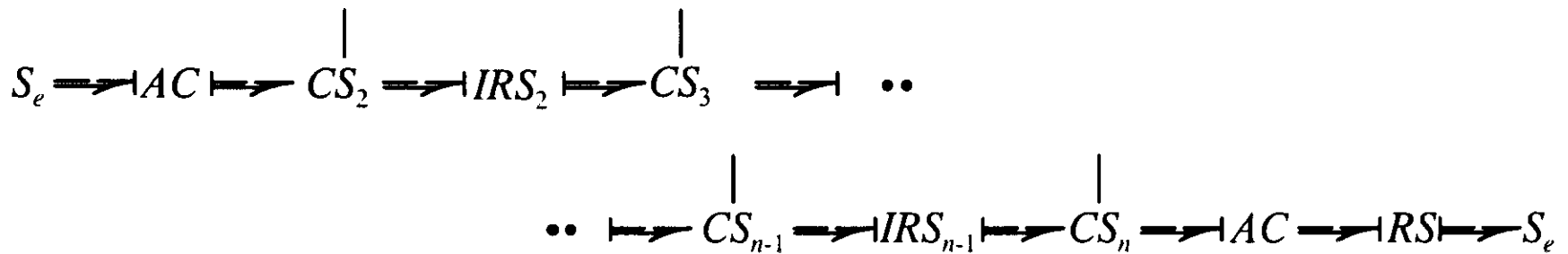
$$p_i^- = (p_{i-1} + p_i)/2; \quad p_i^+ = (p_i + p_{i+1})/2$$

$$\frac{dp_i}{dt} = \left( \frac{A_i + A_{i+1}}{2} \right) (P_i - P_{i+1}) - F_{w,i} + \frac{(p_i^-)^2}{\rho_i A_i L^2} + \frac{(p_i^+)^2}{\rho_{i+1} A_{i+1} L^2}$$

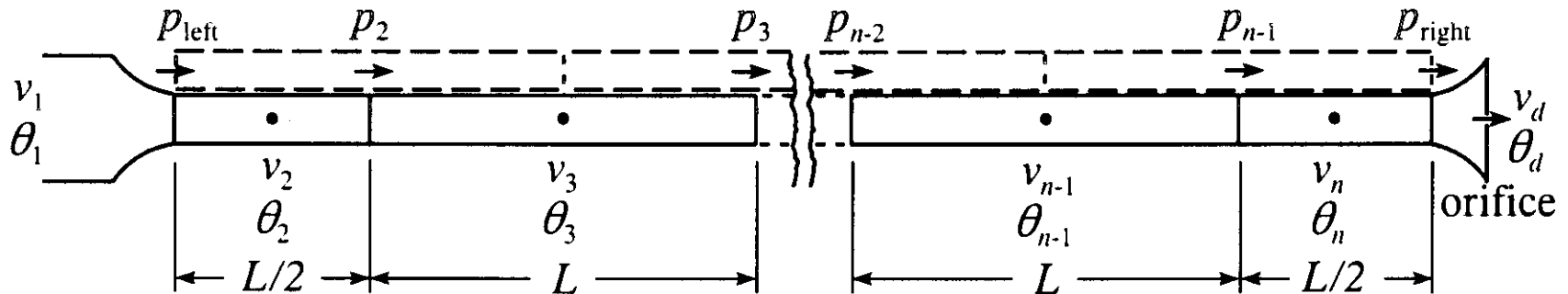
Partial mixing of fluid within the CS elements, called upwinding, often is used.

# Simulation of refrigeration condenser

A condenser tube has vapor enter at the left and liquid leave at the right after equilibrium is reached. The model below adds a new area change element (AC) at each end, and an orifice at the right. 40 *IRS* and 41 *CS* elements were assumed.

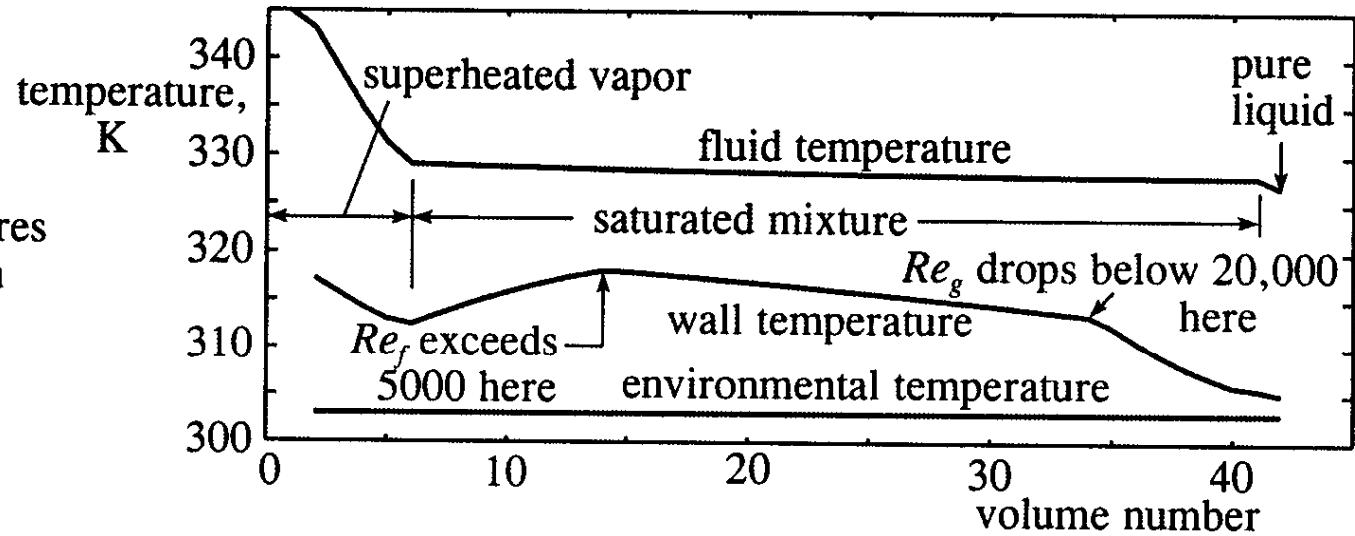


Control volumes for *CS* elements are shown by solid lines;  
control volumes for *IRS* elements are shown by dashed lines.

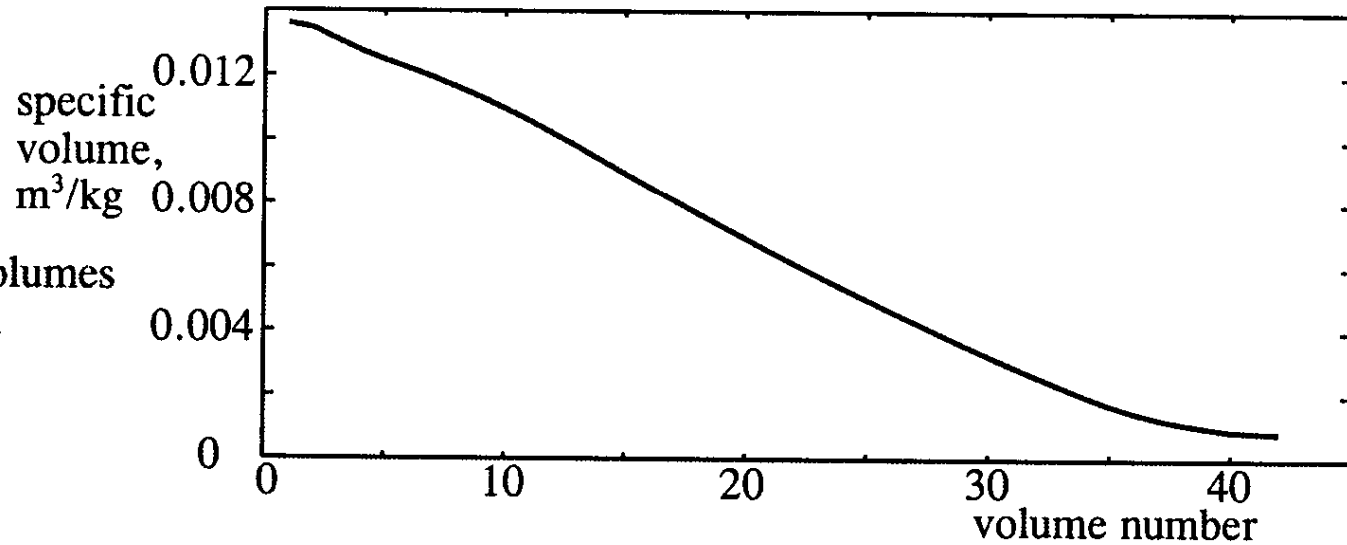


# Simulation results

(a) temperatures at equilibrium

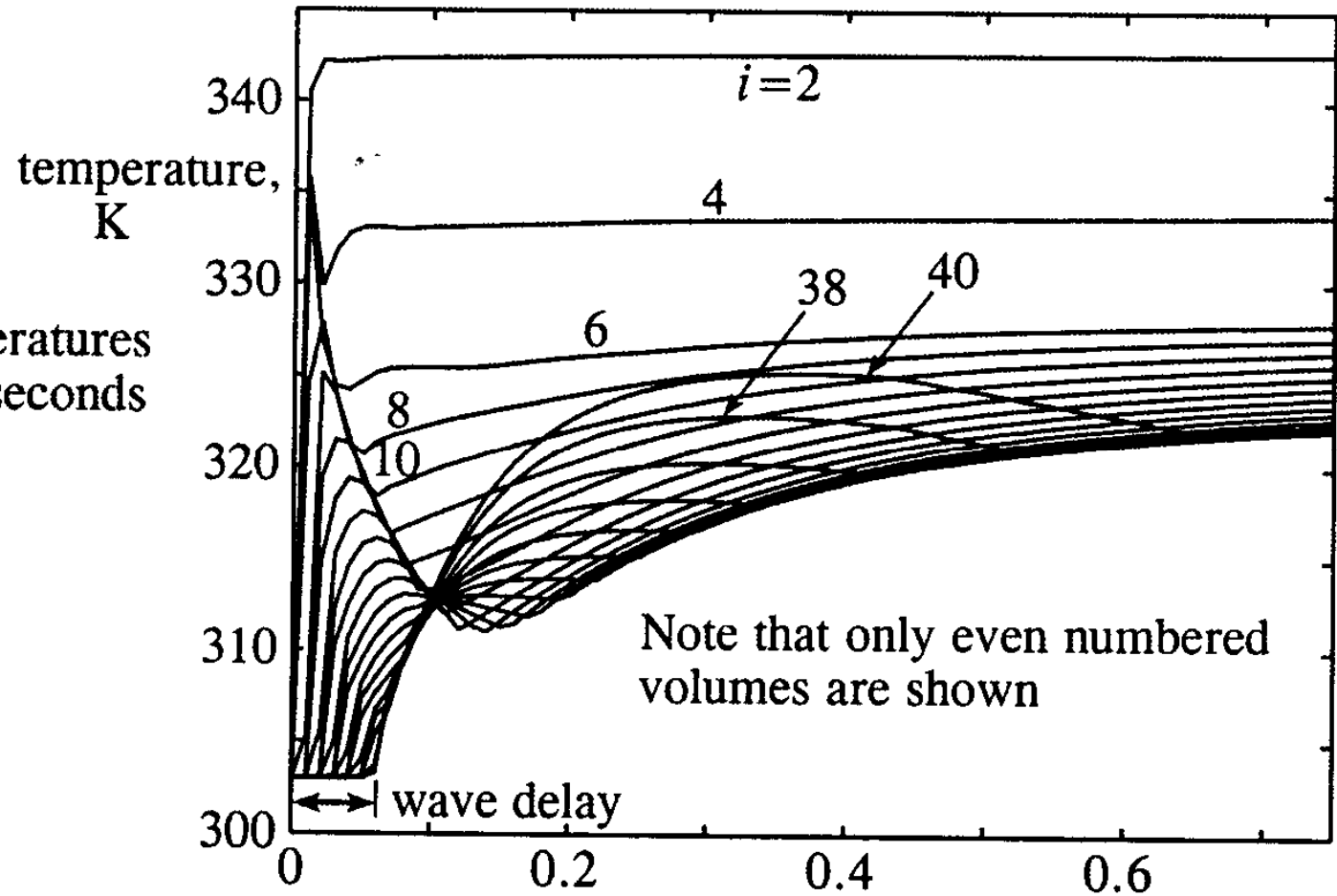


(b) specific volumes at equilibrium



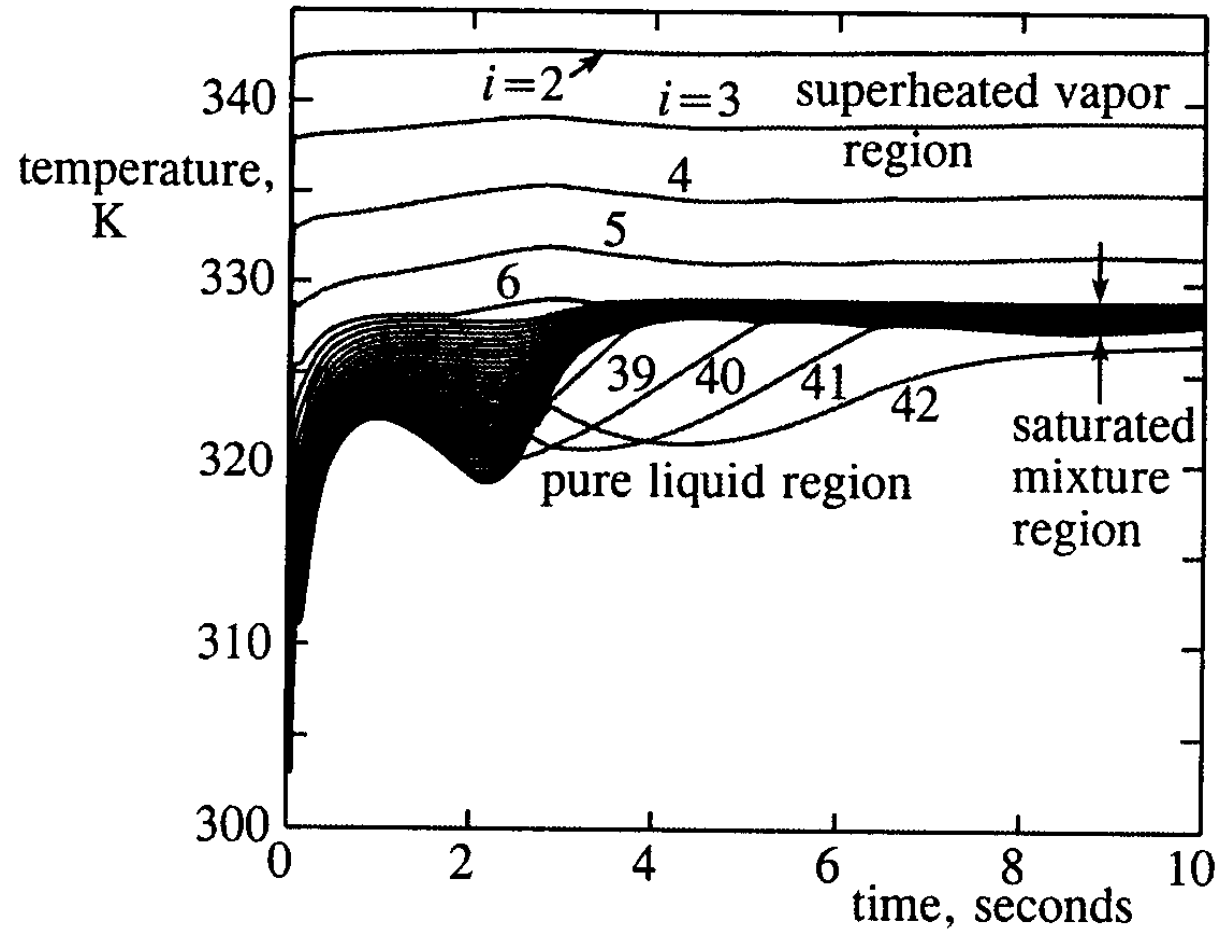
# Simulation results, continued

(c) fluid temperatures for first 0.75 seconds



# Simulation results, continued

(d) fluid temperature for first 10 seconds



# Part III Evaluation of thermodynamic properties

When formulas in the basic form

$$P = P(\rho, \theta) \quad \text{or} \quad P = P(v, \theta); \quad v \equiv 1/\rho; \quad c_v^0 = c_v^0(\theta)$$

are used, the following equations for computing internal energy and entropy can be derived and implemented:

$$u = \int_{\theta_0}^{\theta} c_v^0(\theta) d\theta + \int_0^{\rho} \frac{1}{\rho^2} \left[ P - \left( \frac{\partial P}{\partial \theta} \right)_{\rho} \right] d\rho + u_0; \quad h = u + Pv,$$

$$s = \int_{\theta_0}^{\theta} \frac{c_v^0(\theta)}{\theta} d\theta - R \ln \rho + \int_0^{\rho} \frac{1}{\rho^2} \left[ \rho R - \left( \frac{\partial P}{\partial \theta} \right)_{\rho} \right] d\rho + s_0.$$

For the Helmholtz form  $\psi = \psi(\rho, \theta)$

there results

$$s = - \left( \frac{\partial \psi}{\partial \theta} \right)_{\rho}; \quad u = \left[ \frac{\partial(\psi\tau)}{\partial \tau} \right]_{\rho}; \quad h = u + P/\rho,$$

$$P = \rho^2 \left( \frac{\partial \psi}{\partial \rho} \right)_{\tau}; \quad \tau \equiv 1/\theta.$$

# Evaluation of thermodynamic properties, cont.

These formulas apply only in the single-phase region. This includes, on its boundary, the saturated liquid and saturated vapor states. They are the only pair of states that, at a given temperature, have the same pressure and Gibbs function. They are awkward to compute, however, but fortunately equations of the following form are available or can be deduced once for all, where  $f$  means liquid and  $g$  means vapor:

$$\rho_f = \rho_f(\theta); \quad \rho_g = \rho_g(\theta).$$

In the two-phase region, equations of the form  $P_{sat} = P_{sat}(\theta)$

have been deduced, which allow  $s$ ,  $h$  and  $u$  to be evaluated:

$$\left( \frac{s - s_g}{v - v_g} \right)_{\theta} = \left( \frac{\partial P}{\partial \theta} \right)_{sat},$$

$$h = h_g + (s - s_g)\theta; \quad u = h - Pv.$$

# Thermodynamic properties of refrigerants

As an example, most refrigerants are characterized as

$$P = \frac{R\theta}{v-b} + \sum_{i=2}^5 \frac{1}{(v-b)^i} (A_i + B_i\theta + C_i e^{-K\theta/\theta_c}) + \frac{A_6 + B_6\theta + C_6 e^{-K\theta/\theta_c}}{e^{\alpha v} (1 + ce^{\alpha v})},$$

$$\ln P_{sat} = F_1 + \frac{F_2}{\theta} + \frac{F_3}{\theta^2} + F_4 \ln \theta + F_5 \theta + F_6 \theta^2 + F_7 \theta^3 + \frac{F_8 (F_9 - \theta)}{\theta} \ln[(F_9 - \theta) F_{10}],$$

$$\rho_f = \sum_{i=1}^5 [D_i X^{(i-1)/3} + D_6 X^{1/2} + D_7 X^2]; \quad X \equiv 1 - \theta / \theta_c,$$

$$\rho_g = \rho_c (\theta / \theta_c)^{E_{25}} \exp \left[ \sum_{i=-10}^{13} E_{i+11} X^{i/3} \right],$$

$$c_v^0 = \sum_{i=1}^7 G_i \theta^{i-3}.$$

Coefficients are published to about 9 significant numbers. It is usually necessary to deduce analytically the enthalpy, internal energy, entropy and, when they apply, the saturated vapor and liquid values of these properties. Many partial derivatives of these properties often are needed, also, if iteration is to be avoided.

# Thermodynamic properties of water

The Helmholtz free energy of water (as given by Keenan) is

$$\psi = \psi_0(\theta) + R\theta[\ln\rho + \rho Q(\rho, \tau)]; \quad \tau \equiv 1000 / \theta,$$

$$\psi_0 = \sum_{i=1}^6 C_i / \tau^{i-1} + C_7 \ln\theta + C_9 \ln\theta / \tau,$$

$$Q = (\tau - \tau_c) \sum_{j=1}^7 (\tau - \tau_{aj})^{j-2} \left[ \sum_{i=1}^8 A_{ij} (\rho - \rho_{aj})^{i-1} + e^{-E\rho} \sum_{i=9}^{10} A_{ij} \rho^{i-9} \right],$$

Saturation  
properties:

$$P_{sat} = P_c \exp \left\{ \left( \frac{\theta_c}{\theta} - 1 \right) \sum_{i=1}^8 F_i [a(\theta - \theta_c)]^{i-1} \right\},$$

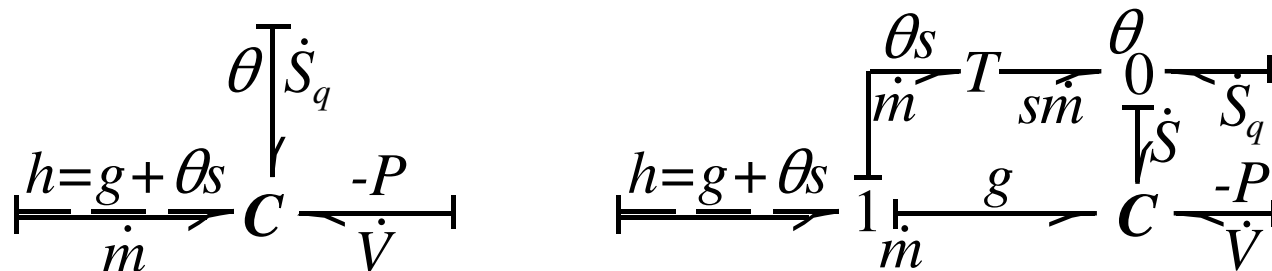
$$\rho_f = \rho_c \left[ 1 + \sum_{i=1}^8 D_i (1 - \theta / \theta_c)^{i/3} \right],$$

$$\rho_g = \left( \frac{\theta}{\theta_c} \right)^{E_1} \exp \left[ \sum_{i=2}^{15} E_i \left( 1 - \frac{\theta}{\theta_c} \right)^{(i-1)/3} \right].$$

# Part IV Chemical reactions

Lumped models with well-mixed reactants are assumed in this introduction. Chemical kinetics also must deal with mixing and diffusion phenomena.

The idea of using the Gibbs free energy,  $g$ , and the product  $\theta s$  as the efforts on a convection bond (recall that  $h = g + \theta s$ ) has special merit when more than one species is involved. The bond graph for the energy stored with a single species that has been used so far, shown on the left below, can be reticulated as shown on the right:



With the energy function  $\mathcal{V} = \mathcal{V}(S, V, m)$ , the output efforts are found from

$$\theta = \left( \frac{\partial \mathcal{V}}{\partial S} \right)_{V, m} ; \quad -P = \left( \frac{\partial \mathcal{V}}{\partial V} \right)_{S, m} ; \quad g = \left( \frac{\partial \mathcal{V}}{\partial m} \right)_{V, S} ; \quad h = g + \theta s.$$

# Chemical reactions, continued

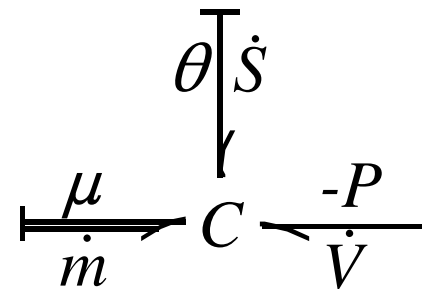
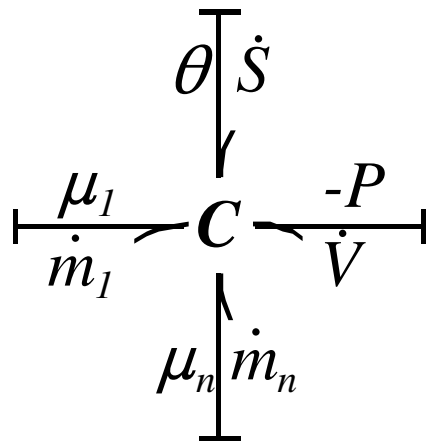
With more than one species present, the equations become

$$\mathcal{V} = \mathcal{V}(S, V, m_1, m_2, m_3, \dots),$$

$$\theta = \left( \frac{\partial \mathcal{V}}{\partial S} \right)_{V, m_1, m_2, \dots} ; \quad -P = \left( \frac{\partial \mathcal{V}}{\partial V} \right)_{S, m_1, m_2, \dots} ; \quad \mu_i = \left( \frac{\partial \mathcal{V}}{\partial m_i} \right)_{V, S, m_{j \neq i}} .$$

Each  $\mu_i$  is a partial Gibbs free energy known as a **chemical potential**.

This suggests the bond graphs below; the one on the right uses the conventional vector bond notation.

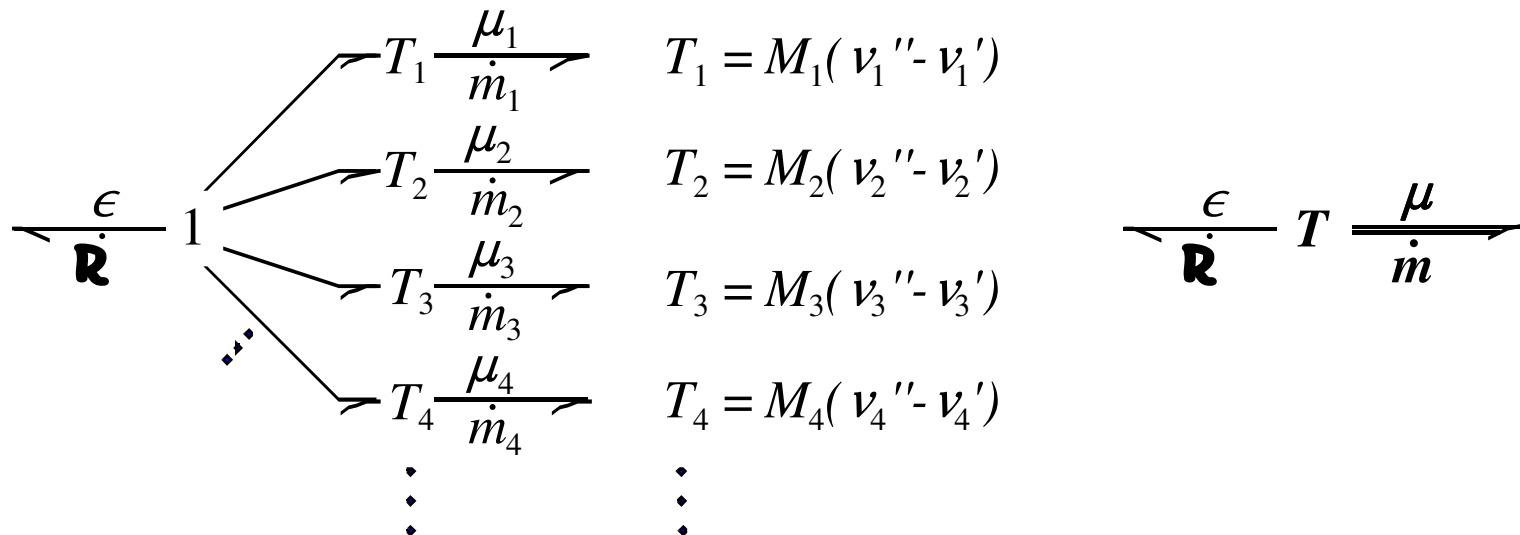


# Chemical reactions, continued

A chemical reaction can be described by  $\sum_{i=1}^n v_i' \bar{\rho}_i \Leftrightarrow \sum_{i=1}^n v_i'' \bar{\rho}_i$ ,

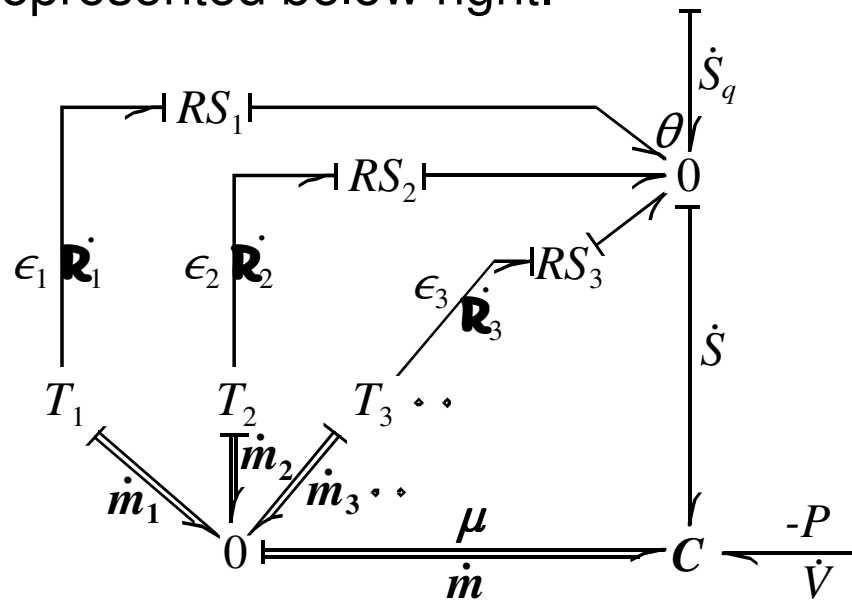
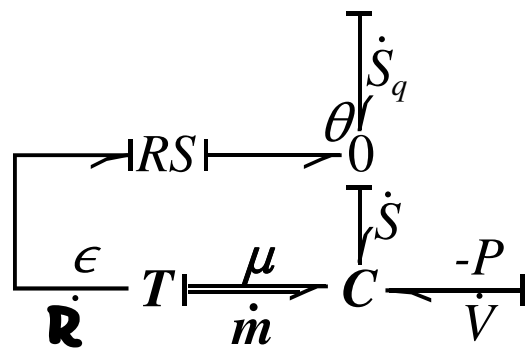
where the molar density and the **stoichiometric coefficients**, respectively, are  $\bar{\rho}_i, v_i', v_i''$ .

The bond graph below represents this constraint and the proper relation to the **reaction force** or **chemical affinity**,  $\epsilon$ , and the reaction rate,  $dR/dt$ , with the transformer moduli  $T_i = M_i(v_i'' - v_i')$ , in which the  $M_i$  are the molar masses.



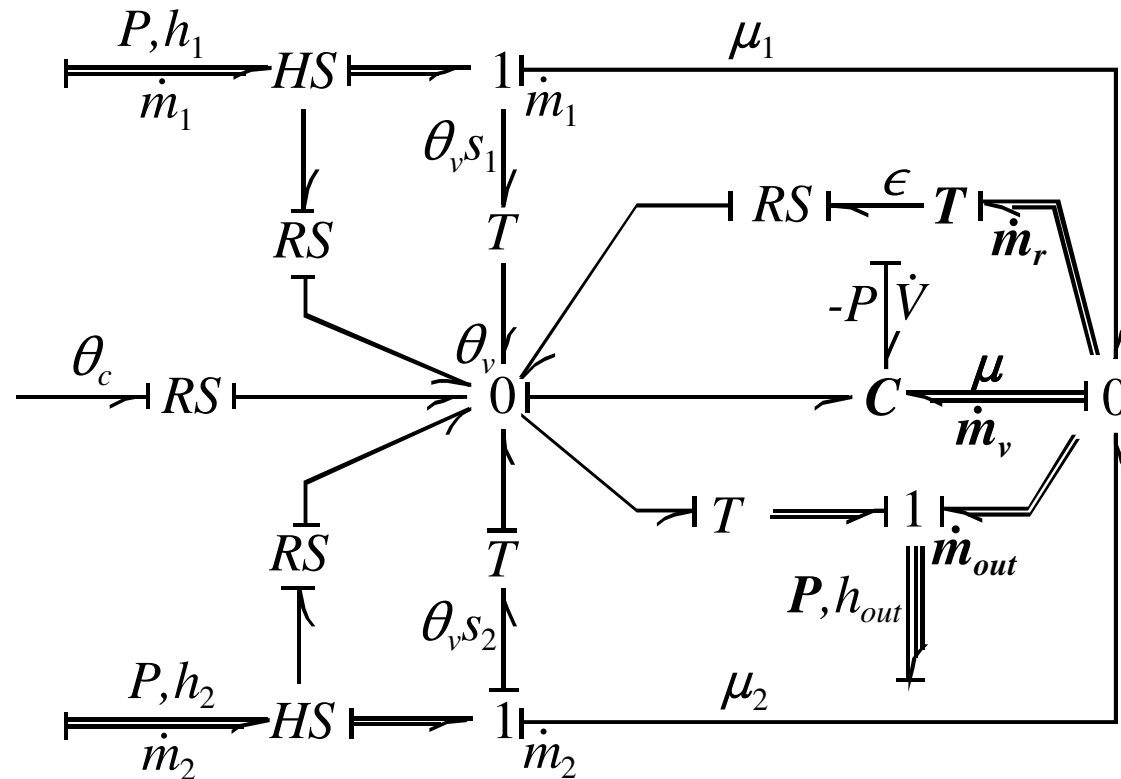
# Chemical reactions, continued

Reaction rates are controlled by the law of mass action with its forward and backward reaction rate coefficients. These can be represented in an RS element, leading to the complete bond graph below left for a one-step chemical reaction in a closed container. Most reactions are in fact not one-step; they are represented below right.



# Chemical reactions, continued

The previous descriptions omit mass flows. Two in-flows and two out-flows are included in the bond graph below. The tank is still assumed to be well-mixed, which is the principal limitation.



# References

To download this PowerPoint presentation from the Internet, go to [lehigh.edu/~inmech](http://lehigh.edu/~inmech), click faculty and, under emeritus, Forbes Brown. It is in the second list of files with the date 1/1/2007; just click on the file name Plenary 2007 ICBGM.

Details on the topics surveyed here are most readily found in the speaker's book *Engineering System Dynamics, A Unified Graph-Centered Approach*, Second Ed., CRC Press, 2007, mostly in Section 9.7 and Chapter 11. Related material is included in the first edition of this book and the following selected papers by the speaker:

“Convection Bond Graphs,” J. Franklin Institute, v 328 n 5/6, 1991, pp. 871-886.

“Simulating Thermodynamic Systems,” ICBGM'99, pp.196-201.

“Non-iterative Evaluation of Multiphase Thermal Compliances in Bond Graphs,” *Proc. Institution of Mechanical Engineers Part I*, v 216 n-1 (2002) pp. 13-20.

## References, continued

“Kinetic Energy in Convection Bond Graphs,” *ICBGM '03*, pp. 191-197.

### **Other authors (highly selected) and possibly biased comments:**

Thoma, J.U. “Entropy and Mass Flow for Energy Conversion,” *J. Franklin Inst.*, v 299 n 2 (1975), pp. 89-96. *Important early work.*

Karnopp, D., “State Variables and Pseudo Bond Graphs for Compressible Thermodynamic Systems,” *ASME Trans., J. Dyn. Systems, Measurement and Control*, v 101 (1979), pp.201-204. *Widely cited; especially useful for linear heat conduction; not true bond graphs.*

Shoureshi, R.A. et al, “Applications of Bond Graphs to Thermofluid Processes and Systems,” *ibid*, v 94 n 4 (1985), pp.241-245. *Important concepts, broad scope.*

## References, continued

Thoma, J.U. and B. Ould Bouamama, *Modeling and Simulation in Thermal and Chemical Engineering, A Bond Graph Approach*, Springer-Verlag, Berlin, 2000. *This is the culmination of a series of publications by Thoma, and represents a major competitive style to the speaker's.*

Greifeneder, J. and Cellier, F.E., "Modeling Convective Flows Using Bond Graphs" and "Modeling Multiphase Systems Using Bond Graphs," *ICBGM '01*, pp. 276-291. *Conventional bond approach. Double-counts pressure work;  $g$  should be replaced by  $u$  as a bond graph effort.*

Pedersen, E., "Modeling Multicomponent Two-Phase Thermodynamic Systems Using Pseudo Bond Graphs," *ibid*, pp. 257-263. *Uses Pen Robinson equation of state for multicomponent gases. Nice reference list.*

## References, continued

Breedveld, P., "Paynter's Verdical State Equation in Integral Causal Form, *ibid*, pp. 27-32. *Improvement on van-der-Waals state equation for gases.*

Reitman, J., "Bond Graphs for Convective Heat Transfer Elements," *ICBGM '05*, pp. 262-270. *Special approach for ideal gases.*