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Basic thermodynamics of energy conversions and energy use

by

B. Eriksson[†], K.E. Eriksson[*†] and G. Wall[*]

[*]Institute of Theoretical Physics, Göteborg
[†]Centre for Interdisciplinary Studies of the
Human Condition, Göteborg University,
S-412 85 Göteborg, Sweden

Institute of Theoretical Physi
Fack
S-402 20 GÖTEBORG
Sweden

Abstract

Thermodynamic relations of basic importance for the understanding of energy conversions and energy use are reviewed. Since physically there is no principle difference between use of energy resources and use of material resources the discussion covers a basic description of natural resources in general. The basic concept is negentropy (Schrödinger) or exergy (Rant). Examples are given of how negentropy or exergy are consumed in various irreversible processes.

The thermodynamic concepts are closely related to the information concept of cybernetics (Shannon, Weaver, Brillouin, Jaynes). "Information" has several connotations however (Attali) and a direct relation between negentropy (or exergy) and information exists only on the basic (physical) level. A brief discussion is also given of information and its relations to exergy at the more complex levels.

Dissipative systems (Prigogine) live on exergy obtained from processing energy and/or matter. Such systems as well as information processing systems are usually protected from the outer world by some "shell" and connected to other systems by a "network" of transport and/or communication lines. Some elementary examples are given of how a system can grow under various conditions and how systems compete for resources. Also some basic conceptual tools for system analysis are introduced.

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1 Introduction

The aim of this paper is to give a fairly comprehensive review of the thermodynamic elementa that are needed to describe energy flows and conversions. The central concept in this context is exergy, the mechanical work that could be obtained from a system in a given environment. Exergy is energy with a quality measure built-in.

In 1953 Z. Rant(1) suggested that the term exergy (Exergie) be used to denote "technische Arbeitsfähigkeit"(2,3). A clear definition was given by H.D. Baehr(4):

"Die Exergie ist der unbeschränkt, d.h. in jede andere Energieform umwandelbare Teil der Energie". (Exergy is the totally convertible part of the energy, i.e. that part which may be converted into any other energy form.)

The exergy concept embodies other thermodynamic quantities(5,6) like enthalpy or free energy (Gibbs or Helmholtz). Unlike energy, exergy is thus a quantity which can be destroyed or - as we prefer to say - consumed. Exergy is consumed whenever entropy is created, i.e. in any irreversible process.

As will be shown the exergy of a system is a measure of its contrast against the surrounding environment. Therefore a high local concentration of a chemical element or compound which is rare elsewhere carries exergy.

Exergy is thus a useful general concept for an accounting of natural resources(7) (what is usually called energy resources as well as material resources).

More generally exergy is the fuel for any system that converts energy and matter in a metabolic process(8). Such a system dissipates energy i.e. consumes exergy and it must be in an exergy flow in order to keep functioning. Geophysical-geochemical systems and living systems on the earth get their exergy from the continuous solar radiation.

In the steering of exergy flows certain regulatory functions are sometimes carried out by special <u>information</u>-processing systems. Information[9-11] is a concept with several levels of complexity.[12] as will be discussed in the paper.

On a basic physical level information (I_{phys}) and negentropy ($\underline{\Sigma}$) are identical,[6,10]

$$\Sigma = k' \, I_{phys} \qquad k' = \text{fundamental constant}$$

and simply related to exergy (E) through

$$E = T_o \Sigma = k' T_o I_{phys}$$

where T_o is the environment temperature.

When a piece of matter, for instance a piece of iron ore is reduced into iron it gains exergy. The exergy spent in the process exceeds the exergy stored in the material by approximately one order of magnitude. If it is then made into steel of a certain composition and structure defined within certain tolerance limits and further formed into a tool of a certain shape, also within certain tolerance limits, then it is given a definite amount of information ΔI.[13] Usually a lot more exergy (by many orders of magnitudes) than $k' T_o \Delta I$ is spent in the industrial process.[13]

What has been said so far clearly indicates that the exergy and information concepts could play important roles in a physical description of economic processes.[14]

On the more complex levels information may still be strongly related to exergy but in more indirect ways. And "man liveth not by bread (i.e. exergy) alone"[15] but has also a mental and intellectual (i.e. information-processing) life.

Our starting point is the basic concepts and the basic relations of thermodynamics and the underlying theory, statistical mechanics.(16) The exergy concept is introduced in section 2 and related to other thermodynamic concepts. In Section 3 the simple example of an ideal monatomic gas is demonstrated. Conversions between heat and mechanical energy are reviewed in Section 4. Examples of exergy losses in energy conversions are given in Section 5. Currents and densities of thermodynamical quantities are introduced in Section 6, including the exergy current and exergy consumption rate density. General features of systems near equilibrium are reviewed in Section 7 including the evolution towards a steady state. Section 8 discusses very briefly the dependence of the efficiency in a conversion process on the rate of conversion, i.e. the power transmitted. The relation between exergy and information is briefly reviewed in Section 9. A characteristic temperature is defined in terms of the exergy spent per bit in an information transfer process. A brief discussion is given in Section 10 of exergy-consuming (i.e. dissipating) systems placed in an energy flow. In Section 11 the complex information concept is analyzed at several levels and in various contexts with the relations to exergy kept in mind. Section 12, finally, deals with coupled dissipative systems.

Little or nothing is new in this paper. Important but more advanced topics like the theory of states far from equilibrium are not treated. Still we hope it may be of some use to have in one paper fundamental material collected from many different sources.

2 Work available from a system in a given environment

Consider a system A in a surrounding system A_0, assumed to be homogeneous and to be large in comparison to A (Fig. 1).

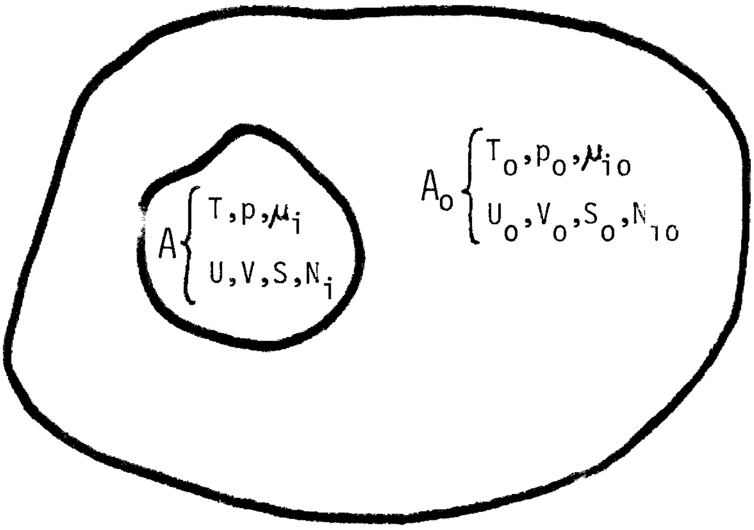

Fig. 1 A system A in an environment A_0.

The "environment" A_0 can then be characterized by its intensive parameters T_0, p_0, μ_{io} (temperature, pressure, chemical potentials). The corresponding parameters for A are T, p and μ_i. (For the moment A is also assumed to be homogeneous.) The extensive parameters for A are U, V, S and N_i (energy, volume, entropy and the number of molecules of different chemical components). The extensive parameters of A_0 are assumed to be large in comparison to the corresponding quantities for A

$$\begin{cases} U \ll U_0 \\ V \ll V_0 \\ N_i \ll N_{io} \end{cases} \tag{1}$$

The combined system A + A_0 is assumed to be isolated (no exchange of matter or energy with the external world) apart from work W extracted from A,

$$\begin{cases} dU + dU_0 + dW = 0 \\ dV + dV_0 = 0 \\ dN_i + dN_{io} = 0 \end{cases} \tag{2}$$

Interaction between A and A_0 can take place in a controlled way through the boundary surface of A. Since A is small (eq.(1)) this does not change the intensive parameters of A_0,

$$\begin{cases} dT_0 = 0 \\ dp_0 = 0 \\ d\mu_{io} = 0 \end{cases} \tag{3}$$

The entropy differential of the environment A_0 is 16)

$$\begin{aligned} dS_0 &= \frac{1}{T_0}\left(dU_0 + p_0 dV_0 - \sum_i \mu_{i0}\, dN_{i0}\right) = \\ &= -\frac{1}{T_0}\left(dU + p_0 dV - \sum_i \mu_{i0}\, dN_i\right) - \frac{dW}{T_0} \end{aligned} \tag{4}$$

where we have used (2). The total entropy differential then is 17)

$$\begin{aligned} dS^{(tot)} &= dS_0 + dS = \\ &= -\frac{1}{T_0}\left(dU + p_0 dV - T_0 dS - \sum_i \mu_{i0}\, dN_i\right) - \frac{dW}{T_0} \end{aligned} \tag{5}$$

This may be written as

$$dS^{(tot)} = -\frac{1}{T_0}\left(dE + dW\right) \tag{6}$$

where we have introduced the exergy E,[5,6]

$$\boxed{E = U + p_0 V - T_0 S - \sum_i \mu_{io} N_i} \tag{7}$$

If we use the relation[16]

$$U = TS - pV + \sum_i \mu_i N_i \tag{8}$$

in (7) we get

$$E = S(T - T_0) - V(p - p_0) + \sum_i N_i(\mu_i - \mu_{io}) \tag{9}$$

which shows that E vanishes for equilibrium ($T = T_0$; $p = p_0$, $\mu_i = \mu_{io}$).

Assume now that A evolves towards equilibrium with its environment A_0 without doing any work ($dW = 0$). The exergy is then changed from E to 0 and the total entropy is changed from $S^{(tot)}$ to $S^{(tot)}_{equilibr}$. Integrating (6) we then get

$$S^{(tot)}_{equilibr} - S^{(tot)} = -\frac{1}{T_0}(-E)$$

and thus

$$E = T_0\left(S^{(tot)}_{equilibr} - S^{(tot)}\right)$$

Defining now negentropy Σ as

$$\boxed{\Sigma = S^{(tot)}_{equilibr} - S^{(tot)}} \tag{10}$$

we then have

$$\boxed{E = T_0 \Sigma \geq 0} \tag{11}$$

The exergy of A thus is T_0 multiplied by the negentropy for A and its environment A_0. We note that in the definition of exergy (7) only the intensive parameters of A_0 appear.

During the process through which equilibrium is attained the exergy thus changes by -E (from E to 0). Let the total entropy increase be ΔS and let the total work extracted be W. Then the integrated version of (6) is

$$\Delta S = -\frac{1}{T_0}(-E + W) \tag{12}$$

or

$$W = E - T_0 \Delta S \tag{13}$$

Since

$$\Delta S \geq 0 \tag{14}$$

with equality only for a reversible process we have

$$\boxed{W \leq E} \tag{15}$$

i.e. the exergy E is the maximal amount of work that may be extracted from A in its process of reaching equilibrium with its environment (A_0).

We may subtract from (7) the corresponding equation at equilibrium. Since E vanishes at equilibrium we then find

$$E = U - U_{eq} + p_0(V - V_{eq}) - T_0(S - S_{eq}) - \sum_i \mu_{i0}(N_i - N_{i\,eq}) \tag{16}$$

which is a useful equation for practical computations of the exergy

In special cases exergy differences reduce to differences of other, better known, thermodynamic potentials, as described in the following table.

Table I. Relations between differences in exergy and in other thermodynamic potentials.[5]

Case	Relevant thermodynamic potential = X		
	$\Delta E=\Delta X$	Definition of X	Usually named
$\Delta N_i=0$	$\Delta E=\Delta G_o$	$G_o=U+p_oV-T_oS$	
$\Delta N_i=0;\Delta V=0$	$\Delta E=\Delta F_o$	$F_o=U-T_oS$	
$\Delta N_i=0;\Delta S=0$	$\Delta E=\Delta H_o$	$H_o=U+p_oV$	
$\begin{cases}\Delta N_i=0\\ T=T_o;p=p_o\end{cases}$	$\Delta E=\Delta G$	$G=U+pV-TS$	Gibb's free energy
$\begin{cases}\Delta N_i=0;\Delta V=0\\ T=T_o\end{cases}$	$\Delta E=\Delta F$	$F=U-TS$	Helmholtz' free energy
$\begin{cases}\Delta N_i=0;\Delta S=0\\ p=p_o\end{cases}$	$\Delta E=\Delta H$	$H=U+pV$	enthalpy

It may be of interest to consider the case of a system A in a local environment A_L which in its turn is embedded in a global environment (Fig. 2). We may then define a "local" exergy

$$E_L = U + p_L V - T_L S - \sum_i \mu_{iL} N_i \qquad (17)$$

which is related to the "global" exergy

$$E = U + p_o V - T_o S - \sum_i \mu_{io} N_i \qquad (7)$$

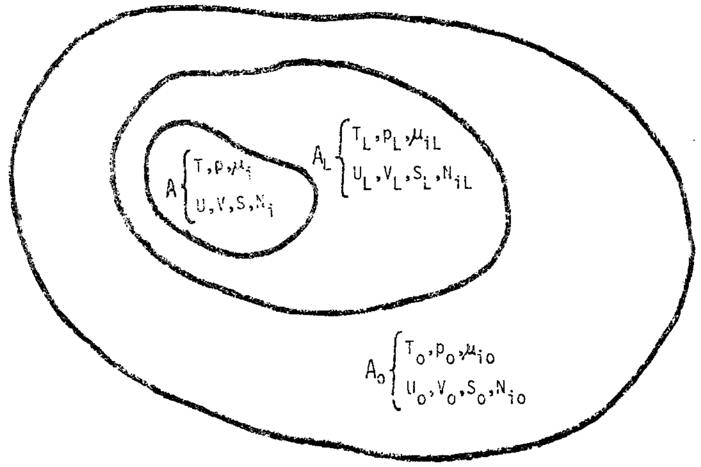

Fig. 2 A system A in a local environment A_L in an environment A_o.

through

$$E = E_{Lo} + E_L \tag{18}$$

where E_{Lo} gives the contribution due to the deviation of the local environment from the global one,

$$E_{Lo} = S(T_L - T_o) - V(p_L - p_o) + \sum_i N_i(\mu_{iL} - \mu_{io}) \tag{19}$$

which is the exergy expression (9) for A with the intensive parameters of A_L replacing those of A. However E_{Lo} is not an exergy function. For instance it is clearly not positive definite.

The exergy or negentropy may be said to be a measure of the contrast of a system against an average "gray" background (see equations (9) and (11)). It is therefore natural that these concepts are closely tied to information theory (Section 10 below). The case of a spatial exergy distribution will be treated in Section 6.

3 Example: The exergy of an ideal monatomic gas[7)]

Consider an ideal monatomic gas enclosed in a container in an environment of the same gas. To determine the exergy we use (16). In any text-book on statistical mechanics we find for this case

$$\begin{cases} V = \dfrac{NkT}{p} \\ U = \frac{3}{2} NkT \\ S = S_{eq} + Nk\left(\frac{3}{2} \ln \dfrac{T}{T_0} + \ln \dfrac{V}{V_{eq}}\right) \end{cases} \qquad (20)$$

where N is now the total number of molecules and

$$\begin{cases} V_{eq} = \dfrac{NkT_0}{p_0} \\ U_{eq} = \frac{3}{2} NkT_0 \end{cases} \qquad (21)$$

We vary volume and temperature and keep N constant,

$$N = N_{eq} \qquad (22)$$

We then get

$$E = NkT_0 \left[\frac{3}{2}\left(\frac{T}{T_0} - 1 - \ln \frac{T}{T_0}\right) + \frac{V}{V_{eq}} - 1 - \ln \frac{V}{V_{eq}}\right] \qquad (23)$$

Expressed in terms of relative deviations from equilibrium

$$\begin{cases} t = \dfrac{T - T_0}{T_0} \\ v = \dfrac{V - V_{eq}}{V_{eq}} = \dfrac{Tp_0}{T_0 p} - 1 \end{cases} \qquad (24)$$

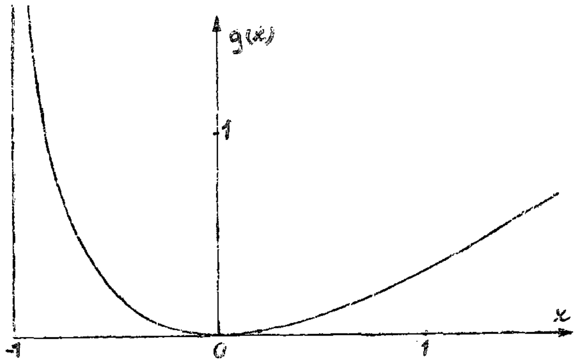

Fig. 3 The function g(x) = x - ln(1+x).

the exergy is

$$E = NkT_0 \left[\frac{3}{2} g(t) + g(v)\right] \qquad (25)$$

where g(x) is the function (Fig. 3)

$$g(x) = x - \ln(1+x) \qquad (26)$$

The divergence3) at x = -1 is connected to an extention of Stirling's formula in the derivation of (20) and (21) outside its range of validity.

4 Efficiency in conversions between heat and mechanical energy[18)]

Let us now consider only a small part of the evolution towards equilibrium. We write (6) in difference form and suppress the superscript "(tot)",

$$\Delta S = -\frac{1}{T_0}(\Delta E + \Delta W) \qquad (27)$$

If we extract work from A (Fig. 4) which then loses exergy

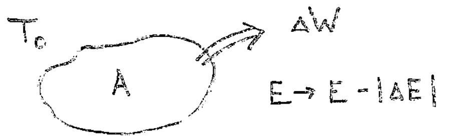

Fig. 4 The system as a heat engine.

$$\begin{cases} \Delta W > 0 \\ \Delta E < 0 \end{cases} \qquad (28)$$

(A is a heat engine), then (27) gives us

$$\Delta W = |\Delta E| - T_0 \Delta S \quad \text{(heat engine)} \qquad (29)$$

and we can define the efficiency as

$$\eta = \frac{\Delta W}{|\Delta E|} = 1 - T_0 \frac{\Delta S}{|\Delta E|} \quad \text{(heat engine)} \qquad (30)$$

If instead work is done on A (Fig. 5), which then gains exergy

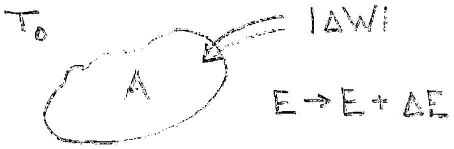

Fig. 5 The system as a heat pump or as a refrigerator.

$$\begin{cases} \Delta W < 0 \\ \Delta E > 0 \end{cases} \qquad (31)$$

A is a heat-pump or a refrigerator, then (27) gives

$$\Delta E = |\Delta W| - T_0 \Delta S \quad (\text{heat-pump/refrigerator}) \tag{32}$$

and the efficiency is

$$\eta = \frac{\Delta E}{|\Delta W|} = 1 - T_0 \frac{\Delta S}{|\Delta W|} \quad (\text{heat-pump/refrigerator}) \tag{33}$$

The efficiency defined in (30) or (33) is the exergy efficiency (or "second law" efficiency) which never exceeds unity,

$$\eta \leq 1 \tag{34}$$

For many forms of energy, the exergy content is very close to the energy content. This does not hold for heat. It may therefore be of interest to consider heat transfer to and from a system A.

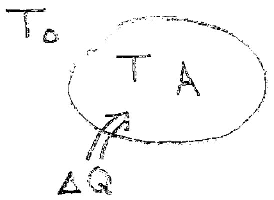

Fig. 6 Heat transfer to A.

Let us first assume that the amount ΔQ of heat is transferred to A (Fig. 6) at constant volume and chemical composition ($\Delta V = \Delta N_i = 0$). Then

$$\Delta S_A = \frac{\Delta Q}{T} \tag{35}$$

is the entropy change of A and

$$\Delta E = \Delta Q - T_0 \Delta S_A = \Delta Q \left(1 - \frac{T_0}{T}\right) \tag{36}$$

is the change in exergy of A. The total negentropy change is

$$\Delta \Sigma = -\left(\frac{\Delta Q}{T} - \frac{\Delta Q}{T_0}\right) = \Delta Q \left(\frac{1}{T_0} - \frac{1}{T}\right)$$

in agreement with (11). The ratio (Carnot factor)

$$q = \frac{\Delta E}{\Delta Q} = 1 - \frac{T_0}{T} \tag{37}$$

is a quality measure of the transferred heat (heat of temperature T in an environment of temperature T_0).

If instead $T<T_0$ the exergy of A can be increased through cooling, i.e. ΔE and ΔQ are of opposite signs. Now $|\Delta E/\Delta Q|$ may be regarded as a quality index for the "cold" $-\Delta Q$ added to or extracted from A,

$$q = \left|1 - \frac{T_0}{T}\right| \tag{38}$$

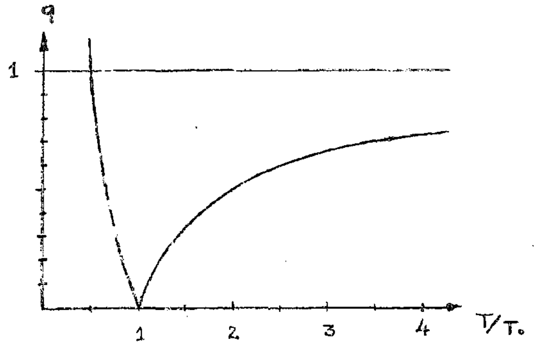

Fig. 7 Quality index for heat (or cold) as a function of ratio of temperature to environment temperature.

The energy efficiency (or "first law efficiency") η_{en} is for the cases considered in the beginning of this section (Fig. 8)

Heat engine ($\Delta Q(T-T_0)>0; \Delta W>0$):

$$\eta_{en} = \frac{\Delta W}{|\Delta Q|} = q\frac{\Delta W}{|\Delta E|} = q\eta \tag{39}$$

It is important to note that a heat engine working with a cold sink at very low temperature may may have a very high energy efficiency.

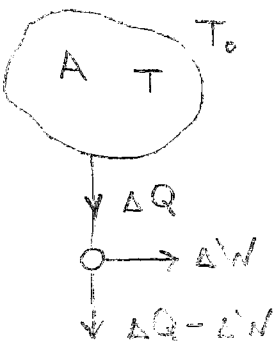

Fig. 8 Energy flows for heat engine ($\Delta Q(T-T_0)$ and $\Delta W>0$) or heat pump/refrigerator ($\Delta Q(T-T_0)$ and $\Delta W<0$).

Heat pump or refrigerator ($\Delta Q(T-T_0)<0; \Delta W<0$):

$$\eta_{en} = \frac{|\Delta Q|}{|\Delta W|} = \frac{1}{q}\frac{\Delta E}{|\Delta W|} = \frac{\eta}{q} \tag{40}$$

5 Some examples of energy conversions and exergy losses 18)

Since the entropy increase ΔS is of main importance in determining the efficiency η (see (30) and (33)) we shall consider a few processes and determine ΔS and η.

i) Heat conduction between two (otherwise) insulated heat capacitors, 1 and 2, joined by an insulated heat conductor ($T_1 > T_2 > T_0$) as shown in Fig. 9.

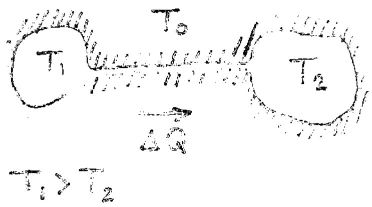

Fig. 9 Heat conduction.

The total entropy change is

$$\Delta S = \Delta Q \left(\frac{1}{T_2} - \frac{1}{T_1}\right) \tag{41}$$

where the transferred heat ΔQ is small enough not to change the temperatures appreciably.

The energy quality for the heat capacitors are

$$q_i = 1 - \frac{T_0}{T_i} \quad (i = 1, 2) \tag{42}$$

The exergy changes are

$$\begin{cases} \Delta E_1 = -\Delta Q\left(1 - \frac{T_0}{T_1}\right) \\ \Delta E_2 = \Delta Q\left(1 - \frac{T_0}{T_2}\right) \end{cases} \tag{43}$$

The exergy loss thus is

$$-\Delta E = -(\Delta E_1 + \Delta E_2) = T_0 \Delta Q \left(\frac{1}{T_2} - \frac{1}{T_1}\right) = T_0 \Delta S \tag{44}$$

The efficiency is

$$\eta = \frac{\Delta E_2}{|\Delta E_1|} = \frac{T_1 (T_2 - T_0)}{T_2 (T_1 - T_0)} \tag{45}$$

ii) A phase transition (Fig. 10) at temperature $T>T_0$ and pressure p_0 with negligible volume change. Heat is extracted from the process at temperature T. Let the phases be 1 and 2 and assume $\mu_1>\mu_2$. Use small letters u_i, v_i, s_i, e_i $(i=1,2)$ for average energy, volume, entropy and exergy per molecule. With

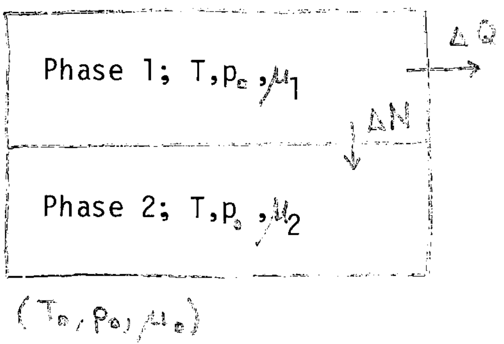

Fig. 10 Phase transition.

$$v_1 = v_2 \tag{46}$$

we then get from (8) and (9)

$$\begin{cases} u_i = Ts_i - p_0 v_i + \mu_i \\ e_i = (T-T_0)s_i + \mu_i - \mu_0 \end{cases} \tag{47}$$

Since

$$-\Delta N_1 = \Delta N_2 = \Delta N \tag{48}$$

we then have

$$-\Delta Q = \Delta N(u_2 - u_1) = [-(Ts_1 + \mu_1) + Ts_2 + \mu_2]\,\Delta N \tag{49}$$

where ΔQ is the heat given to the environment. The total entropy change is

$$\Delta S_1 + \Delta S_2 + \frac{\Delta Q}{T} = -(s_2 - s_1)\,\Delta N +$$

$$+ \frac{1}{T}(Ts_1 + \mu_1 - Ts_2 - \mu_2)\,\Delta N = \frac{\mu_1 - \mu_2}{T}\,\Delta N$$

and the exergy loss per molecule in transition is

$$\frac{T_0}{T}(\mu_1 - \mu_2) \tag{50}$$

The efficiency in the transfer of exergy from phase 1 to phase 2 and the environment is then

$$\eta = 1 - \frac{(T_0/T)(\mu_1 - \mu_2)}{e_1} = 1 - \frac{(T_0/T)(\mu_1 - \mu_2)}{(T - T_0)s_1 + \mu_1 - \mu_0} \qquad (51)$$

iii) <u>A chemical reaction</u> at similar conditions (no volume change and heat taken out at reaction temperature T). Let the reaction be

$$\nu_A A + \nu_B B \rightarrow \nu_C C + \nu_D D \qquad (52)$$

Then

$$\begin{cases} \Delta N_A = -\nu_A \Delta \Xi \\ \Delta N_B = -\nu_B \Delta \Xi \end{cases} \qquad \begin{cases} \Delta N_C = \nu_C \Delta \Xi \\ \Delta N_D = \nu_D \Delta \Xi \end{cases} \qquad (53)$$

where $\Delta\Xi$ is the net number of elementary reactions. The entropy change in the system is

$$\Delta S = (-\nu_A s_A - \nu_B s_B + \nu_C s_C + \nu_D s_D)\Delta \Xi \qquad (54)$$

The heat released is

$$\begin{aligned} \Delta Q &= -\Delta U = -T\Delta S + \sum_i \mu_i \Delta N_i = \\ &= [\nu_A(Ts_A + \mu_A) + \nu_B(Ts_B + \mu_B) - \nu_C(Ts_C + \mu_C) - \nu_D(Ts_D + \mu_D)]\Delta \Xi \end{aligned} \qquad (55)$$

The total entropy increase is

$$\frac{\Delta Q}{T} + \Delta S = \frac{A}{T}\Delta \Xi \qquad (56)$$

where A is the affinity of the reaction,

$$A = \nu_A \mu_A + \nu_B \mu_B - \nu_C \mu_C - \nu_D \mu_D \qquad (57)$$

The exergy delivered from the initial state is

$$-(\Delta E_A + \Delta E_B) = (T - T_0)(\nu_A S_A + \nu_B S_B) + \nu_A(\mu_A - \mu_{A0}) + \nu_B(\mu_B - \mu_{B0}) \tag{58}$$

and similarly for the exergy going into the final state $\Delta E_C + \Delta E_D$. The total exergy loss is thus

$$\Delta E = \Delta E_A + \Delta E_B + \Delta E_C + \Delta E_D + \left(1 - \frac{T_0}{T}\right)\Delta Q$$

which by (58) and (55) amounts to

$$\Delta E = -T_0\left(\frac{A}{T} - \frac{A_0}{T_0}\right)\Delta \xi \tag{59}$$

$$A_0 = \nu_A \mu_{A0} + \nu_B \mu_{B0} - \nu_C \mu_{C0} - \nu_D \mu_{D0}$$

which may be compared with the entropy production (56). When $A_0=0$, ΔE is $-T_0$ times the entropy production as expected. When $A_0 \neq 0$ we have an environment which deviates from final equilibrium even if there is a strong barrier against the reaction. This explains the extra term in (59).

The efficiency is (for $A_0=0$)

$$\eta = 1 - \frac{A(T_0/T)}{(T - T_0)(\nu_A S_A + \nu_B S_B) + \nu_A(\mu_A - \mu_{A0}) + \nu_B(\mu_B - \mu_{B0})} \tag{60}$$

6 Local exergy consumption[19]

Consider a system of several chemical components of molecular mass m_i and $n_i(\underline{x},t)$ molecules per unit mass. The mass density of each component is

$$\rho_i(\underline{x},t) = m_i n_i(\underline{x},t)\rho(\underline{x},t) \tag{61}$$

where the total mass density is

$$\rho(\underline{x},t) = \sum_i \rho_i(\underline{x},t) \tag{62}$$

For each component we introduce a velocity field

$$\underline{v}_i(\underline{x},t) = \underline{v}(\underline{x},t) + \underline{u}_i(\underline{x},t) \tag{63}$$

where $\underline{v}$ is the center-of-mass velocity,

$$\begin{cases} \rho\underline{v} = \sum_i \rho_i \underline{v}_i & (64) \\ \sum_i \rho_i \underline{u}_i = 0 & (65) \end{cases}$$

The hydrodynamic time derivative (i.e. for a volume element along its center-of-mass motion) is

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \underline{v}\cdot\underline{\nabla} \tag{66}$$

Conservation of mass implies the continuity equation,

$$\frac{\partial \rho}{\partial t} + \underline{\nabla}\cdot(\rho\underline{v}) = 0 \tag{67}$$

Let a be the amount per unit mass of some extensive quantity such that ρa is the corresponding density and $\rho a\underline{v}$ the corresponding current density. Then because of (67) the source of this quantity is

$$\frac{\partial(\rho a)}{\partial t} + \underline{\nabla}\cdot(\rho a \underline{v}) = \rho \frac{da}{dt} \tag{68}$$

For the special choice a = v where

$$v = \rho^{-1} \tag{69}$$

is the specific volume, we find

$$\frac{dv}{dt} = v\,\underline{\nabla}\cdot\underline{v} \tag{70}$$

If there is a chemical reaction going on with ν_i molecules of the i th component produced (for $\nu_i > 0$; for $\nu_i < 0$ $|\nu_i|$ molecules consumed) in each elementary reaction we have a stoichiometric relation

$$\sum_i m_i \nu_i = 0 \tag{71}$$

We also have a balance equation for each chemical component,

$$\frac{\partial \rho_i}{\partial t} + \underline{\nabla}\cdot(\rho_i \underline{v}_i) = \nu_i m_i \xi \tag{72}$$

where ξ is the reaction rate density.

The different molecular species may be subject to different external forces. Let the external force per unit mass for the i th component be $\underline{f}_i(\underline{x},t)$ and let the corresponding potential energy per unit mass be $\omega_i(\underline{x},t)$. The force per unit mass of the mixture $\underline{f}(\underline{x},t)$ is determined by

$$\rho \underline{f} = \sum_i \rho_i \underline{f}_i \tag{73}$$

and similarly for the total potential energy per unit mass ω,

$$\rho \omega = \sum_i \rho_i \omega_i \tag{74}$$

There are also internal forces described by the pressure tensor which we assume to be of the form, valid for a fluid,

$$P_{ij} = p\delta_{ij} + \pi_{ij} \tag{75}$$

where p is the hydrostatic pressure and where

$$\pi_{ij} = \pi_{ji} \tag{76}$$

The first term in (75) is the elastic term whereas the second term is a <u>dissipative</u> term leading to entropy production. At equilibrium therefore $\pi_{ij}=0$.

The equation of motion for a volume element is the balance equation for momentum

$$\rho \frac{d\underline{v}}{dt} = \rho \underline{f} - \underline{\nabla} \cdot \underline{\underline{P}} \tag{77}$$

or

$$\frac{\partial(\rho \underline{v})}{\partial t} + \underline{\nabla} \cdot (\rho \underline{v} \underline{v}) = \rho \underline{f} - \underline{\nabla} \cdot \underline{\underline{P}} \tag{78}$$

where a dyadic notation is used for P_{ij} and $v_i v_j$. For the time derivative of the kinetic energy density we get from this

$$\frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho \underline{v}^2\right) = -\underline{\nabla} \cdot \left(\tfrac{1}{2}\rho \underline{v}^2 \underline{v}\right) - \underline{v} \cdot (\underline{\nabla} \cdot \underline{\underline{P}}) + \rho \underline{v} \cdot \underline{f} \tag{79}$$

The kinetic energy current density is

$$\underline{\underline{P}} \cdot \underline{v} + \left(\tfrac{1}{2}\rho \underline{v}^2\right) \underline{v} \tag{80}$$

and the source of kinetic energy thus is

$$\begin{aligned} \frac{\partial}{\partial t}\left(\tfrac{1}{2}\rho \underline{v}^2\right) + \underline{\nabla} \cdot \left(\underline{\underline{P}} \cdot \underline{v} + \tfrac{1}{2}\rho \underline{v}^2 \underline{v}\right) &= \\ = \underline{\underline{P}} : (\underline{\nabla} \underline{v}) + \rho \underline{v} \cdot \underline{f} \end{aligned} \tag{81}$$

For the potential energy of each chemical component we have the balance equation

$$\frac{\partial}{\partial t}(\rho_i \omega_i) + \nabla\cdot(\rho_i \omega_i \underline{v}_i) = -\rho_i \underline{f}_i \cdot \underline{v}_i \tag{82}$$

with the sum

$$\frac{\partial}{\partial t}(\rho\omega) + \underline{\nabla}\cdot\left(\sum_i \rho_i \omega_i v_i\right) = -\rho\,\underline{f}\cdot\underline{v} - \sum_i \rho_i \underline{f}_i\cdot\underline{u}_i \tag{83}$$

Here we have used (73) and (74). For the sum of (81) and (83) we get

$$\begin{aligned}&\frac{\partial}{\partial t}\left[\rho\left(\tfrac{1}{2}\underline{v}^2+\omega\right)\right] + \underline{\nabla}\cdot\left[\underline{\underline{P}}\cdot\underline{v} + \tfrac{1}{2}\rho\,\underline{v}^2\underline{v} + \sum_i \rho_i\omega_i\underline{v}_i\right] = \\ &= \underline{\underline{P}}:(\underline{\nabla}\,\underline{v}) - \sum_i \rho_i \underline{f}_i\cdot\underline{u}_i\end{aligned} \tag{84}$$

Besides kinetic energy and potential energy we have an internal energy density ρu and a corresponding current density

$$\rho u\,\underline{v} + \underline{w} \tag{85}$$

where the first term is the convection flow and the second term is the conduction flow (<u>heat flow</u>). The continuity equation expressing over all energy conservation then is

$$\begin{aligned}&\frac{\partial}{\partial t}\left[\rho\left(\tfrac{1}{2}\underline{v}^2+\omega+u\right)\right] + \\ &+\underline{\nabla}\cdot\left[\underline{\underline{P}}\cdot\underline{v} + \tfrac{1}{2}\rho\,\underline{v}^2\underline{v} + \sum_i \rho_i\omega_i\underline{v}_i + \rho u\,\underline{v} + \underline{w}\right] = 0\end{aligned} \tag{86}$$

Subtracting (84) from this we obtain for the internal energy the balance equation

$$\frac{\partial(\rho u)}{\partial t} + \underline{\nabla}\cdot(\rho u\,\underline{v} + \underline{w}) = -\underline{\underline{P}}:(\underline{\nabla}\,\underline{v}) + \sum_i \rho_i \underline{f}_i \underline{u}_i \tag{87}$$

We assume local equilibrium implying that per unit mass we have locally,

$$\begin{cases} u = Ts - pv + \sum_i \mu_i n_i \\ du = T\,ds - p\,dv + \sum_i \mu_i\,dn_i \end{cases} \tag{88}$$

where ρs is the entropy density. Along the centre-of-mass motion one has

$$\frac{du}{dt} = T\frac{ds}{dt} - p\frac{dv}{dt} + \sum_i \mu_i \frac{dn_i}{dt} \tag{89}$$

or

$$\frac{ds}{dt} = \frac{1}{T}\frac{du}{dt} + \frac{p}{T}\frac{dv}{dt} - \sum_i \frac{\mu_i}{T}\frac{dn_i}{dt} \tag{90}$$

We have already by (87), (70) and (72)

$$\begin{cases} \rho\frac{du}{dt} = -\underline{\nabla}\cdot\underline{w} - \underline{\underline{P}}:(\underline{\nabla}\,\underline{v}) + \sum_i \rho_i\,\underline{f}_i\cdot\underline{u}_i \\ \rho\frac{dv}{dt} = \underline{\nabla}\cdot\underline{v} \\ \rho\frac{dn_i}{dt} = \frac{1}{m_i}\left[\frac{\partial\rho_i}{\partial t} + \underline{\nabla}\cdot(\rho_i\underline{v}_i) - \underline{\nabla}\cdot(\rho_i\underline{u}_i)\right] = \nu_i\xi - \underline{\nabla}\cdot(\rho n_i\underline{u}_i) \end{cases} \tag{91}$$

which inserted into (90) give us

$$\begin{aligned} \frac{\partial(\rho s)}{\partial t} + \underline{\nabla}\cdot(\rho s\underline{v}) = &-\frac{1}{T}\underline{\nabla}\cdot\underline{w} - \frac{1}{T}\underline{\underline{\Pi}}:(\underline{\nabla}\,\underline{v}) + \\ &+ \sum_i \frac{\mu_i}{T}\underline{\nabla}\cdot(\rho_i n_i\underline{u}_i) + \frac{A}{T}\xi + \frac{1}{T}\sum_i \rho_i\underline{f}_i\cdot\underline{u}_i \end{aligned} \tag{92}$$

where A is the reaction affinity

$$A = -\sum_i \nu_i\mu_i \tag{93}$$

We may write this as a balance equation for entropy

$$\frac{\partial(\rho s)}{\partial t} + \underline{\nabla}\cdot\underline{j}_s = \sigma \tag{94}$$

where

$$\underline{j}_s = \rho s \underline{v} + \frac{1}{T}\underline{w} - \sum_i \frac{\mu_i}{T}\rho n_i \underline{u}_i \tag{95}$$

may be considered as the *entropy current density* and

$$\begin{aligned}\sigma = {} & \underline{w}\cdot\nabla\left(\frac{1}{T}\right) - \sum_i \rho n_i \underline{u}_i \cdot \left[\nabla\left(\frac{\mu_i}{T}\right) - \frac{m_i}{T}\underline{f}_i\right] - \\ & - \frac{1}{T}\underline{\underline{\Pi}} : (\nabla \underline{v}) + \frac{A}{T}\xi\end{aligned} \tag{96}$$

as the *entropy production density*.

The *exergy density* is in analogy to (7)

$$\rho e = \rho\left(\frac{v^2}{2} + \omega + u\right) + p_0 - \rho\left(T_0 s + \sum_i n_i \mu_{i0}\right) \tag{97}$$

or with (88), (74) and (61)

$$\begin{aligned}e = {} & \frac{1}{2}\underline{v}^2 - v(p - p_0) + s(T - T_0) + \\ & + \sum_i n_i (m_i \omega_i + \mu_i - \mu_{i0})\end{aligned} \tag{98}$$

The exergy current density may similarly be defined as (see (7), (86) and (95))

$$\begin{aligned}\underline{j}_e = {} & \underline{\underline{P}}\cdot\underline{v} + \rho\left(\frac{1}{2}\underline{v}^2\right)\underline{v} + \sum_i \rho_i \omega_i \underline{v}_i + \rho u \underline{v} + \underline{w} - T_0 \underline{j}_s + \\ & + p_0 \underline{v} - \sum_i \rho n_i \mu_{i0} \underline{v}_i\end{aligned} \tag{99}$$

which may be rewritten in a way similar to (98) as

$$\begin{aligned}\underline{j}_e = {} & \rho e \underline{v} + \rho \sum_i n_i m_i \omega_i \underline{u}_i + \\ & + T_0 \left[\underline{w}\left(\frac{1}{T_0} - \frac{1}{T}\right) + \rho \sum_i n_i \underline{u}_i \left(\frac{\mu_i}{T} - \frac{\mu_{i0}}{T_0}\right)\right] + \underline{\underline{P}}\cdot\underline{v}\end{aligned} \tag{100}$$

The *exergy consumption rate density* then is

$$\varepsilon = -\left[\frac{\partial(\rho e)}{\partial t} + \underline{\nabla}\cdot\underline{j}_e\right] \tag{101}$$

Using now (97), (99), (91), (94) and (96) we obtain the final expression for the exergy consumption

$$\begin{aligned}\varepsilon &= T_0\sigma - p_0\underline{\nabla}\cdot\underline{v} - A_0\xi = \\ &= T_0\Big\{\underline{w}\cdot\underline{\nabla}\left(\frac{1}{T}\right) + \sum_i \rho n_i \underline{u}_i\cdot\left[\underline{\nabla}\left(-\frac{\mu_i}{T}\right) + \frac{1}{T}m_i\underline{f}_i\right] - \\ &\quad - \frac{1}{T}\underline{\underline{P}}:(\underline{\nabla}\,\underline{v}) + \left(\frac{A}{T} - \frac{A_0}{T_0}\right)\xi + \left(\frac{p}{T} - \frac{p_0}{T_0}\right)\underline{\nabla}\cdot\underline{v}\Big\}\end{aligned} \tag{102}$$

where

$$A_0 = -\sum_i \nu_i \mu_{i0} \tag{103}$$

Like in (59) the exergy consumption (102) differs from T_0 times the entropy production by a term which involves the environment's affinity A_0 for the chemical reaction under study. In (102) there is also a volume term $-p_0\underline{\nabla}\cdot\underline{v}$. For a fixed closed boundary the integral over this term vanishes.

7 Systems near equilibrium[20)]

As in the previous section we shall assume local equilibrium. Moreover we shall assume that variations of densities, temperature etc. within the system are limited so that certain linear relations may be assumed. As we shall see if such a system has stationary boundary conditions it evolves towards a steady state characterized by minimum entropy production.

We shall let our system be characterized by the variables

$$\alpha_i(\underline{x},t)=\frac{\zeta_i(\underline{x},t)}{\zeta_{i\,eq}}-1;\quad i=0,1,2,\ldots \tag{104}$$

where ζ_i are densities; $\zeta_0=\rho u$ and where $\zeta_{0eq}=(\rho u)_{eq}$ and $\zeta_{ieq}(i=1,2,\ldots)$ are equilibrium values. The corresponding currents ("flows") are

$$\underline{J}_i(\underline{x},t)=\frac{\underline{j}_i(\underline{x},t)}{\zeta_{i\,eq}};\qquad i=0,1,2,\ldots \tag{105}$$

We shall consider the case that there is no net center-of-mass flow, nor any external force and no chemical reaction, i.e. $\underline{v}=0$ and $\xi=0$. Then (86) and (72) read

$$\dot{\alpha}_i+\underline{\nabla}\cdot\underline{J}_i=0 \tag{106}$$

Within the approximations we shall use, the negentropy of our system is (cf Section 3)

$$\Sigma(t)=\int_V d^3x\,\tfrac{1}{2}\,g_{ij}\,\alpha_i(\underline{x},t)\,\alpha_j(\underline{x},t)\geq 0;\quad \sum_{ij}\ \text{understood} \tag{107}$$

where $g_{ij}=g_{ji}$ is a positive definite matrix. Inhomogeneities are characterized by "forces"

$$\underline{X}_i(\underline{x},t)=-\underline{\nabla}\frac{\delta\Sigma}{\delta\alpha_i(\underline{x},t)}=-g_{ij}\,\underline{\nabla}\,\alpha_j(\underline{x},t) \tag{108}$$

which "drive" the system towards equilibrium.

If we are close enough to equilibrium we may assume linear relations between flows and forces

$$\underline{J}_i = \underline{\underline{L}}_{ij}\cdot\underline{X}_j = -(\underline{\underline{L}}_{ik}\, g_{kj})\cdot\nabla\alpha_j \tag{109}$$

where Onsager's relations

$$L_{i\alpha j\beta} = L_{j\beta i\alpha} \tag{110}$$

hold, expressing the principle of detailed balancing, which may be derived from microscopic invariance under time reversal. Moreover $\underline{\underline{L}}_{ij}$ is positive definite.

We can now study the time development of $\alpha_i(\underline{x},\underline{t})$. We get from (106) and (109)

$$\dot{\alpha}_i(\underline{x},t) = -\nabla\cdot\underline{J}_i(\underline{x},t) = \nabla\cdot\underline{\underline{L}}_{ik}\cdot\nabla\, g_{kj}\alpha_j(\underline{x},t) \tag{111}$$

which leads to the following time development

$$\begin{aligned}\alpha_i(\underline{x},t) &= (2\pi)^{-3/2}\int d^3p\; e^{i\underline{p}\cdot\underline{x}}\left(e^{-\underline{p}\cdot\underline{\underline{L}}\cdot\underline{p}\, g t}\right)_{ij}\beta_j(\underline{p})\,;\\ \beta_j(\underline{p}) &= (2\pi)^{-3/2}\int d^3x\; e^{-i\underline{p}\cdot\underline{x}}\,\alpha_j(\underline{x},0)\end{aligned} \tag{112}$$

i.e. an exponential decay of the deviation from equilibrium. This holds when there are no flows that keep the system off equilibrium. In the general case the second equation (112) should be replaced by

$$\beta_j(\underline{p}) = (2\pi)^{-3/2}\int d^3x\; e^{-i\underline{p}\cdot\underline{x}}\left[\alpha_j(\underline{x},0) - \alpha_j^{(0)}(\underline{x})\right] \tag{112'}$$

where $\alpha_j^{(0)}(x)$ is a stationary solution, satisfying the equation

$$\underline{\nabla}\cdot\underline{\underline{L}}\cdot\underline{\nabla}\, g_{kj}\,\alpha_j^{(0)}(\underline{x}) = 0 \tag{113}$$

with the proper boundary conditions. The entropy production is (see (107), (111), (109) and (108))

$$\begin{aligned}\dot{S}(t) &= -\dot{\Sigma}(t) = \int_V d^3x\; g_{ij}\,\alpha_i(\underline{x},t)\,\dot{\alpha}_j(\underline{x},t) = \\ &= -\int_V d^3x\; \alpha^{\sim} g\, \underline{\nabla}\cdot\underline{\underline{L}}\cdot\underline{\nabla}\, g\,\alpha = \int_V d^3x\; \underline{J}_i\cdot\underline{X}_i = \int d^3x\; \underline{X}_i\cdot\underline{\underline{L}}_{ij}\cdot\underline{X}_j\end{aligned} \tag{114}$$

We identify the entropy production density

$$\sigma(\underline{x},t) = \underline{X}_i(\underline{x},t)\cdot\underline{\underline{L}}_{ij}\cdot\underline{X}_j(\underline{x},t) \geqslant 0 \tag{115}$$

The time derivative of the entropy production is

$$\begin{aligned}\ddot{S}(t) &= 2\int_V d^3x\; \underline{X}^{\sim}\cdot\underline{\underline{L}}\cdot\dot{\underline{X}} = 2\int_V d^3x\; \alpha^{\sim} g\, \overset{\leftarrow}{\underline{\nabla}}\cdot\underline{\underline{L}}\cdot\overset{\rightarrow}{\underline{\nabla}}\, g\,\dot{\alpha} = \\ &= -2\int_V d^3x\; \alpha^{\sim} g\, \overset{\leftarrow}{\underline{\nabla}}\cdot\underline{\underline{L}}\cdot\overset{\leftarrow}{\underline{\nabla}}\, g\,\dot{\alpha} = -2\int_V d^3x\; \dot{\alpha}^{\sim} g\,\dot{\alpha}^{\sim} \leqslant 0\end{aligned} \tag{116}$$

When the system is in a stationary flow which can be described by stationary inhomogeneous boundary conditions then the entropy production $\dot{S}$ decreases towards its minimum. Then the system is described by a solution of (113) compatible with the boundary conditions.

8 Exergy losses in energy conversions

Consider an energy conversion characterized by a typical inflow J. The power inflow into the conversion process P_{in} may then be proportional to J. Let us assume that this is the case

$$P_{in} \propto J \tag{117}$$

In the regim where (109) and (115) hold the entropy production, and thus the exergy loss, is proportional to J^2 and thus to P_{in}^2. If further there is a certain power leakage, we have

$$P_{out} = P_{in} \left(1 - \ell - \frac{P_{in}}{P_0}\right) \tag{118}$$

where ℓ is the fraction which is leaking and where P_0 is a power which is characteristic of the exergy consumption. The efficiency is thus[21)]

$$\eta(P_{in}) = 1 - \ell - \frac{P_{in}}{P_0} \tag{119}$$

Clearly (119) may be considered as the first term of a series expansion valid as long as

$$\frac{P_{in}}{P_0} \ll 1 \tag{120}$$

but otherwise independent of the assumptions made in the derivation.

When there is no leakage $(\ell = 0)$

$$\eta(0) = 1 \tag{121}$$

as should be the case for an infinitely slow (adiabatic) process. For a conversion process of non-zero rate, however, there are always inevitable exergy losses due to entropy production.

9 Systems far from equilibrium. Living systems.

A system may be maintained away from equilibrium if it lies in an energy flow and receives energy from one system and gives it away to another. For such a system A (Fig. 11) the inflow of energy (temperature T_1) carries low entropy and the outflow (temperature $T_2 < T_1$) carries high entropy. If the power is W and the average temperature of A is T_0, then the net exergy gain per unit time is

$$T_0 W\left(\frac{1}{T_2} - \frac{1}{T_1}\right) \tag{122}$$

This exergy flow can be used to construct and maintain structures far away from equilibrium.

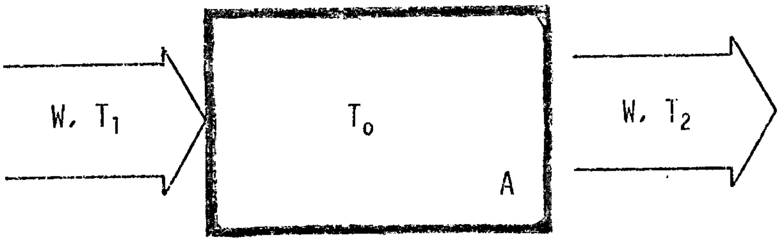

Fig. 11 A system A of average temperature T_0 in an energy flow W.

If a system is in a negentropy (or exergy) flow 8) and if self-catalytic processes are possible then fluctuations may be used as starting points for producing structure and order out of a more chaotic state. 19,22) This is the way life once began on earth. 23) The description of such phenomena, however, fall outside the scope of this article.

A simple way of helping a system which involves self-catalytic processes is to close it within a shell of some sort. A living cell is an obvious example of this.

The net exergy flow to the earth (Fig. 12) amounting to $\approx 1.2 \cdot 10^{17}$ W[*] drives the geophysical system and the biosphere.

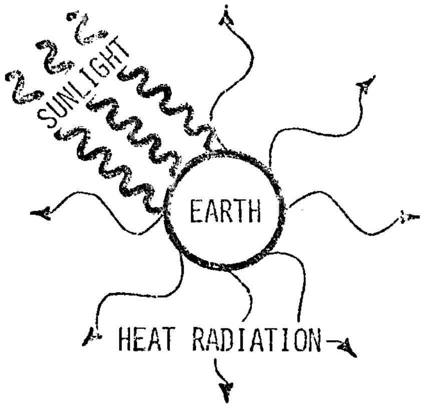

Fig. 12 The SUN-EARTH-SPACE system.

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[*] corresponding to $4 \cdot 10^{37}$ bits/s.[6]

10 Exergy, negentropy and information

The negentropy for a system in classical statistical mechanics is defined as

$$\Sigma = k \sum_n (P_n \ln P_n - P_n^{(0)} \ln P_n^{(0)}); \quad k = \text{Boltzmann's const.} \qquad (123)$$

Here P_n is the probability of finding the system in the state (phase-space cell) labelled by n. Further $P_n^{(0)}$ are the equilibrium probabilities, i.e. the probabilities maximizing the entropy, so that

$$S = -k \sum_n P_n \ln P_n \leq S^{(0)} = -k \sum_n P_n^{(0)} \ln P_n^{(0)} \qquad (124)$$

under the actual constraints like given total values or average values for certain parameters.

In quantum statistical mechanics[16] (123) has to be generalized,

$$\Sigma = k \{ Tr [\rho \ln \rho] - Tr [\rho^{(0)} \ln \rho^{(0)}] \} \qquad (125)$$

where ρ is the density matrix of the system and $\rho^{(0)}$ is the equilibrium density matrix. Here

$$Tr\, \rho = Tr\, \rho^{(0)} = 1 \qquad (126)$$

corresponds to

$$\sum_n P_n = \sum_n P_n^{(0)} = 1 \qquad (127)$$

In quantum mechanics, the concept of a microscopic state is well-defined, for instance in terms of spin states and/or harmonic oscillator wave-functions. Then the information as defined in information theory[9,10] is also well-defined and amounts to (in binary units (bits))

$$I_{phys} = \frac{1}{\ln 2} \left\{ Tr\left[\rho \ln \rho\right] - Tr\left[\rho^{(0)} \ln \rho^{(0)}\right] \right\} \tag{128}$$

Here we have indicated the physical nature of this information concept. Now (123) and (128) differ only by a constant and

$$\boxed{\Sigma = k' \, I_{phys}} \tag{129}$$

where

$$k' = k \ln 2 = 1.0 \cdot 10^{-23} \ J/K \tag{130}$$

Information as defined by (128) means <u>physical information capacity</u> rather than a quantitative measure of an actual message.

Exergy and physical information are thus related through (11) and (128) as[6,11)]

$$\boxed{E = k' T_0 \, I_{phys}} \tag{131}$$

where T_0 is the temperature of the environment.

Quantum mechanics is essential here in defining what should be meant by a physical state. Without quantum mechanics the unit volume of phase-space would be completely arbitrary.

When information is stored or transmitted usually only a limited part of the physical information capacity is being used. There may be groups of many microstates among which no distinction is made. Let Π_J be a projection operator on such a group of microstates, a <u>macrostate</u>, labelled by J and assume J=1,...,K. Then

$$\Pi = \sum_{J=1}^{K} \Pi_J \tag{132}$$

projects on the set of physical states that should be considered. We can now define probabilities

$$\begin{cases} P_J = \dfrac{Tr(\pi_J \rho)}{Tr(\pi \rho)}\,; & \displaystyle\sum_{J=1}^{K} P_J = 1 \\ P_J^{(0)} = \dfrac{Tr(\pi_J \rho^{(0)})}{Tr(\pi \rho^{(0)})}\,; & \displaystyle\sum_{J=1}^{K} P_J^{(0)} = 1 \end{cases} \tag{133}$$

The <u>information</u> contained is

$$I = \frac{1}{\ln 2}\left[\sum_{J=1}^{K} P_J \ln P_J - \sum_{J=1}^{K} P_J^{(0)} \ln P_J^{(0)}\right] \leq I_{phys} \tag{134}$$

Thus the information contained when only macrostates defined by the projectors π_J are considered is obtained from the density operator ρ through the "<u>coarse-graining</u>" procedure (133). Clearly the result generally contains less information than the original probability distribution.

Information is also a convenient measure of <u>physical structure</u>; a certain structure out of all possible structures is chosen and defined within certain tolerance margins.[13,24]

Biological structures maintain and reproduce themselves by transforming energy from one form to another. Thus the exergy of the radiation from the sun is used to build the highly ordered organic materials. The information laid down in the genetic material is developed and transferred from one generation to another. When biological materials, e.g. wood as such or cellulose, are used as construction materials it is in fact organic structures and the information contained therein that are taken advantage of (the chemical term of (7)).

As was emphasized in the previous section exergy has to be spent in any energy conversion process which goes at a finite rate. When a physical structure is being built up some exergy goes into the structure and some is spent in the conversion processes. Also when information is transferred or stored, energy is dissipated, i.e. exergy is spent in the process.

If the exergy spent in an information transfer is E when the amount of information transferred is I then one may define

$$T_{transfer} = \frac{E}{kI} \qquad (135)$$

as a characteristic temperature of the transfer. A requirement that often has to be met is that $T_{transfer}$ must be large enough in order that enough energy is dissipated to ensure irreversibility. This often means that $T_{transfer}$ has to be large compared to T_0 in the sense that11)

$$e^{-T_{transfer}/T_0} << 1 \qquad (136)$$

a condition which is quite favourable since $T_{transfer}/T_0$ appears in a decreasing exponential.

In Table II the characteristic temperatures of different information transfers are indicated. In Fig. 13 an information rate(frequency)-power plot is made for different types of information transfer.

The sensitivity of the retina is such that the human eye functions close to the quantum mechanical limit. Actually we may see just a few quanta. The storage of information in a computer memory has a characteristic temperature about 10^5 times the temperature of sight. On the other hand its time resolution and consequently its speed is better than that of the eye by roughly 10^5. The conclusion is that living beings and computers are efficient in using exergy to receive or transfer information. The biosynthesis of the cell, however, is still several orders of magnitude more efficient.

Electronic circuits, the human ear and eye and biosynthesis of protein are mapped in the logarithmic frequency-power diagram of Fig. 13 where room temperature is marked by a straight line. Ordinarily a process should be well above this line to remain undisturbed by thermal fluctuations (condition (136)). The biosynthesis of protein, however, falls very close to this critical line. Actually the steps from messenger-RNA to protein which take half of the power required would fall below that line. This is possible because as much as 4.3 bits are transferred in each step. The ear and the eye occupy strikingly large areas in the diagram, covering many orders of magnitude. Electronics is probably the best technology we have from an exergy-economic point of view. Still, as Fig. 13 shows, life itself is much more efficient in its use of exergy in constructing biological material.

Table II. Efficiency in information transfer (expressed in characteristic temperature.

	$T_{transfer}$ (K)
Electric typewriter x)	10^{23}
Radio (receiver) x)	$5 \cdot 10^{19}$
Television x)	$2 \cdot 10^{18}$
Computer memory	10^{11}
Human speech	10^{7}
Human ear	10^{6}
Human eye	$5 \cdot 10^{5}$
Protein synthesis in a cell xx) (overall process)	460

x) The data were obtained from ref. 6.

xx) The data were obtained from Lehninger.25)

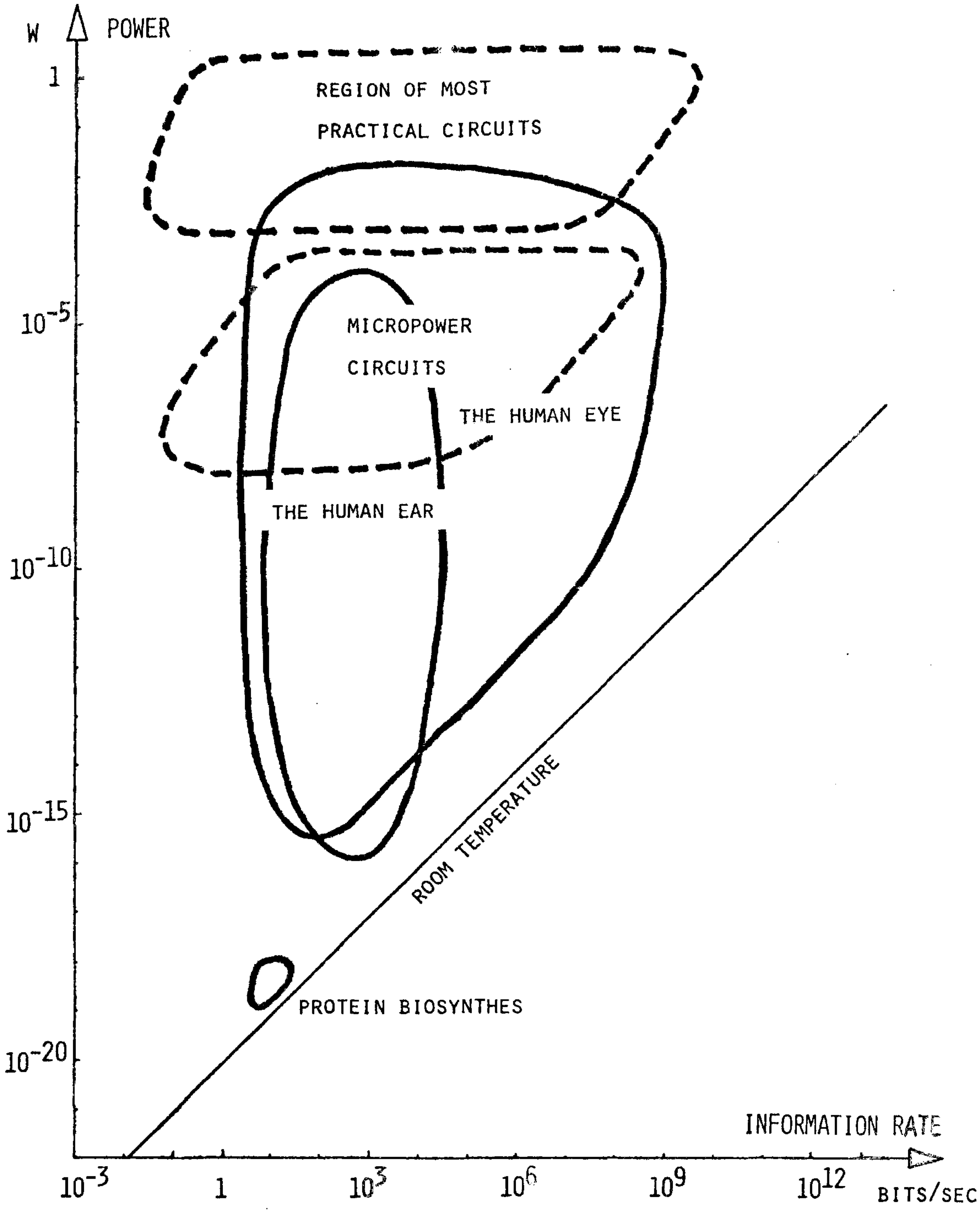

Fig. 13 FREQUENCY-POWER DIAGRAM OF INFORMATION TRANSFER

The minimum power in integrated circuits has been treated by several authors 26, 27) . It has been shown by Brillouin 11) that an elementary process in a circuit, such as a measurement, a storage of one bit, or a logical operation, requires an energy dissipation which is large in comparison with $kT\ 4\cdot 10^{-21}$ J (at room temperature). This is necessary to avoid thermal agitation which is the origin of noise in electric circuits, Brownian motion, etc. The energy value $4\cdot 10^{-21}$ J is indicated by the straight line in the diagram. Information transfer must take place above this line. The protein biosynthes 25, 28) can stay very close to this line because of the fact that in every elementary transfer 4.3 bits of information are exchanged.

11 Levels of information

The concept of information used in the previous section is rather different from the concept of information commonly used. Ordinarily information is required to have some meaning whereas the information concepts that we used in Section 10 were not tied to any meaning. The concept defined by (128) we called physical information. It may carry meaning but it does not necessarily do so.

This shows that it may be useful to distinguish between different levels when dealing with "information". Here we shall follow (rather freely) Jacques Attali[12] and consider information on five different levels as shown in Table III.

Table III. Different levels of information, ordered after decreasing complexity[12]

5. Relational level
4. Semiologic level
3. Semantic level
2. Cybernetic level
1. Physical level

1. The physical level is the simplest one. At this level we have the physical object that carries or transmits the information, like carbon on cellulose (print on paper), acoustic waves or electromagnetic waves, matter of varying units (nucleotides, molecules or bricks) ordered in various patterns.

The physical information capacity is related to exergy through (123). Most of this capacity is not used.

2. The cybernetic level is also conceptually simple. The object carrying information is in a "state", more or less well known, and described by the probability distribution (133) over a set of attainable macrostates. The information contained then is as given by (134).

When information is transmitted or transcribed the exergy spent per bit is a characteristic temperature (135) which depends on the transmission or transcription process (Table II). For the process of reading a book, for instance, the characteristic temperature depends on the lighting and the reading speed.

The digital structure of genetic information (Table IV) and of languages makes these forms of information very directly accessible to a theoretical analysis within information theory (cybernetics).

In a language with N basic signs s_i $(i=1,\dots,N)$ with relative average frequencies ν_i,

$$\sum_{i=1}^{N} \nu_i = 1 \qquad (137)$$

the information content of each individual sign is

$${}^{2}\log \frac{1}{\nu_i} = -\frac{\ln \nu_i}{\ln 2} \qquad (138)$$

Information contained in physical structures like an organism, a tool, a building, or a piece of art, defined within certain tolerance limits can be treated by methods analogous to those used in classical statistical mechanics or the theory of pattern recognition.

Table IV. The genetic code. The four nucleotides ("letters") are arranged in 3-letter "words", each symbolizing and synthesizing one amino acid. The words are arranged in "sentences" defining a chain of amino acids; the order in the chain further defines the spatial structure of the resulting protein. For a protein functioning as an enzyme the geometrical structure is essential for forming an active site which has a specific catalytic effect to steer a certain metabolic reaction.

UUU	Phenylalanine	UCU	Serine	UAU	Tyrosine	UGU	Cysteine
UUC		UCC		UAC		UGC	
UUA	Leucine	UCA		UAA	Ochra	UGA	Umber
UUG		UCG		UAG	Amber	UGG	Tryptophan
CUU	Leucine	CCU	Proline	CAU	Histidine	CGU	Arginine
CUC		CCC		CAC		CGC	
CUA		CCA		CAA	Glutamine	CGA	
CUG		CCG		CAG		CGG	
AUU	Isoleucine	ACU	Threonine	AAU	Asparagine	AGU	Serine
AUC		ACC		AAC		AGC	
AUA		ACA		AAA	Lysine	AGA	Arginine
AUG	Methionine	ACG		AAG		AGG	
GUU	Valine	GCU	Alanine	GAU	Aspartic acid	GGU	Glycine
GUC		GCC		GAC		GGC	
GUA		GCA		GAA	Glutamic acid	GGA	
GUG		GCG		GAG		GGG	

3. Information may be described physically at the first level and cybernetically at the second level. This may sometimes be sufficient to describe a physical structure or a pattern in space and/or time. But usually a message also has a *meaning*. At *the semantic level* we deal with the content, *the information conveyed*. This content may be defined through more or less clear, but seldom explicitely formulated semantic rules.

We shall use this concept in a very broad sense. The semantic rules may be so primitive that they are hardly recognized as semantic rules - as when Pavlov's dogs interpret the sound of their master's bell as meaning food. Or they may be extremely advanced and abstract - as they often are in mathematics or modern physics or in philosophy.

Often the meaning of a message is ambiguous - or it becomes ambiguous if a fraction of it is lost or distorted. To limit this risk one often uses *redundancy* - like the control figure in a registration number or the repetition of a verbal message - often in a slightly varied wording.

Let us consider the case when a piece of information conveyed is a *factual statement*. Then it may be *true* or *false*. No objective criterion exists by which the truth value may be determined. In society or in science there are however operable - and at times very good - *intersubjective truth criteria* that can be employed[x].

When truth or falsity do not apply, other semantic value concepts may be applicable, like: *meaningfulness*, *correctness* or *relevance*. Such concepts are also tied to evaluation criteria or conventions.

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[x] Pilatus' question "What is truth?"[29] may, of course, still not be satisfactorily answered.

A more penetrating analysis of these philosophical questions clearly falls outside the scope of the present paper.

4. Words that we hear or read and which have meaning to us can also carry a more complex connotation reminding us of past experiences or of a body of knowledge. The same can be true of many pieces of information that reach us. Often the wider connotations are of a very personal nature but they are not necessarily so.

When a *sign* or a *symbol* *carries* such a broad *connotation* involving a *body of information* which is not private but which may be *shared by a group of people* or even by masses of people then the sign or symbol carries information at the *semiologic level*. Examples are the Christian cross, a slogan, a piece of music or a quotation from a common literary tradition. Semiologic information often has a strong *emotional component.* Also since the body of information recalled varies between different persons especially in a society with large social differences the semiologic information content may be quite vague. This vagueness makes the study of semiologic information difficult, as often experienced in humanistic sciences.

Signals, also those of a rather primitive nature, exchanged by animals or humans for instance, to express an intention may be quite complex in their connotation and should then be considered as semiologic.

5. At *the relational level* information exchanged between individuals serves to *confirm*, to *suggest*, or to *question relations between those individuals*. Like semiologic information this is a kind of information which goes back in history beyond verbal information, even beyond the appearance of the human race.

Exchange of relational information between animals of the same species has regulatory functions that are important for the survival of the species. These functions are studied in ethology. Clearly relational information has a strong emotional component.

Ethology may be applied to human relations as well although these relations are distorted by society.*)

Much of the information at the levels previously discussed have also relational overtones that may be very delicate to analyze or even to describe.

Relational information is exchanged not only between individual persons but also between individual persons and over-individual persons like a group of people with a strong group ego (strongly correlated wills) or between such over-individual persons.

We conclude this section with a few simpleminded remarks on the relation between exergy and information at the more complex conceptual levels.

Semantic information:
To think or to talk is often cheap in exergy terms or in terms of social consequences whereas the object or process about which information is exchanged may involve large - sometimes virtually unlimited - exergy expenditures and important social changes and connected social costs. To "think or discuss first" (before action) is thus usually advisable or even necessary.

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*)For example there are no ethological regulatory functions that prevent massive killing in a modern war where the victim is no longer a person to the soldier but a mark on a map. Also the victim has little chance of reaching the soldier with any relational message.

Semiologic information:
Structures that are costly in terms of exergy or traditions that involve large expenditures of exergy are sometimes used or practiced at festival occasions to convey a sense of unity among the celebrating people. Often the same semiologic information is also a symbol of the power of the rulers or of the ruling class.

Cathedrals and castles are thus built not only to be used but also to convey semiologic information.

Elegant houses or cars, often expensive to buy and to run, expensive dinners or vacation trips may be pieces of information used by a person or a family to classify one's own rank on the social ladder.

Thus semiologic information of this type is very strongly tied to the exergy consumption.

On the international scene expensive armament plays a role similar to that played by the waste in housing and life style at the personal or family level. To produce the armament vast amounts of exergy are spent and some weapons would - if they were used in their full destructive capacity - mean locally, and maybe globally, an exergy consumption density previously unknown on earth.

Relational information:
Large differences in access to resources, i.e. in freedom of exergy consumption are more easily accepted - and sometimes even considered as natural - if the privileged classes or groups are separated from the deprived classes or groups and if confrontations between representatives of the two sides follow a strict protocol (usually fixed by the privileged sides). In this way exchange of relational information is prevented and the situation may be preserved for a long time. On the global

scene the geographical and cultural separation and the structure of economic interaction are very efficient in separating humankind into consumers and non-consumers. (Fig. 14 illustrates what Harrison Brown[30] calls the fissioning of the human society.)

The relation between exergy and information although simple and direct at the physical level and at the cybernetic level is thus much more involved at the more complex conceptual levels.

To study how exergy and information are turned-over and consumed in natural[31] and societal[32] systems it is very important to identify systems which are principle processors of exergy and/or information and to determine their properties and their mutual interactions - in particular their exchange of exergy and/or information.

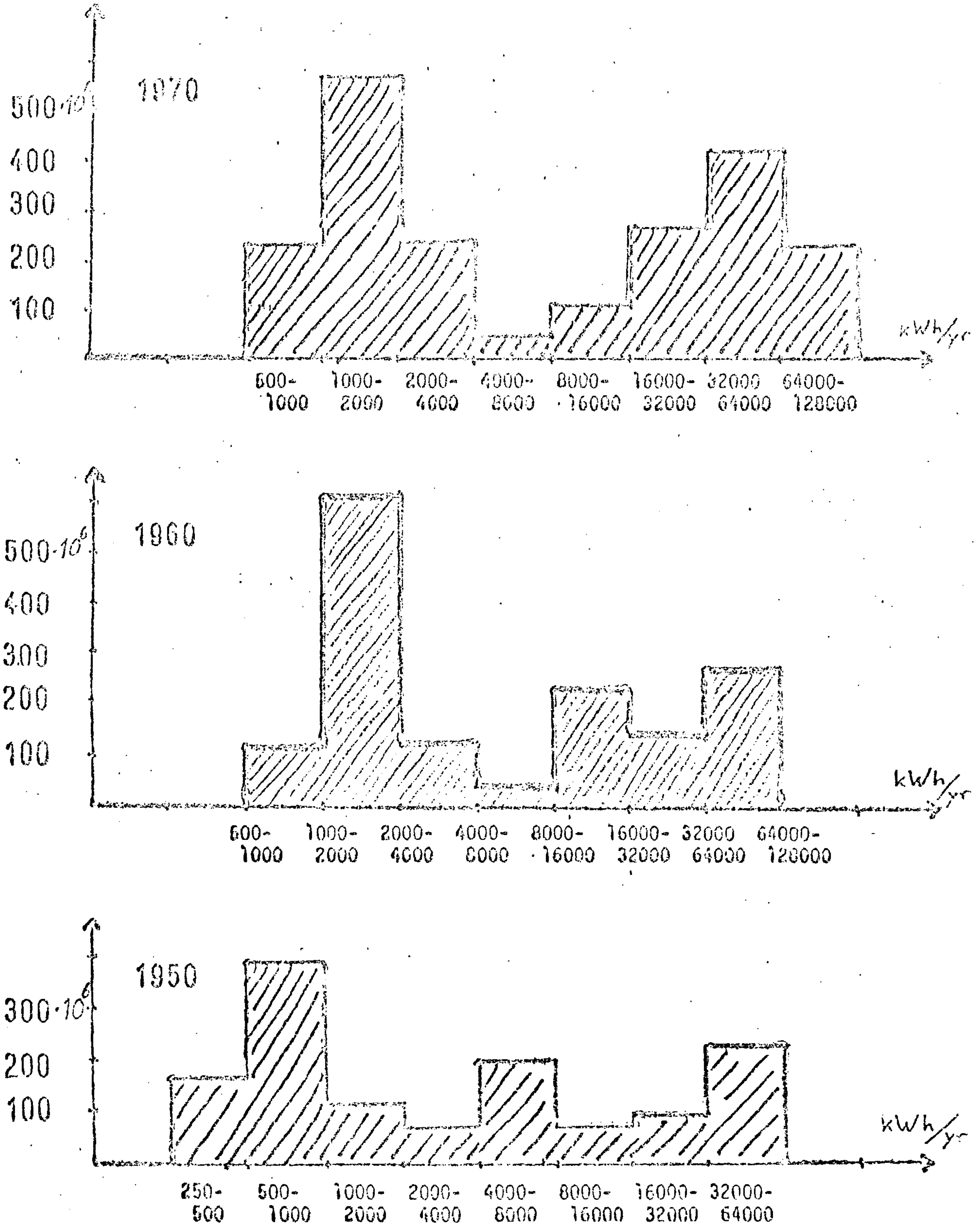

Fig. 3. ENERGY USE PER CAPITA FOR THE WORLD POPULATION
(Harrison Brown, Energy in Our Future, Annual Review of Energy, Vol. 1, 1976)

12 Dissipative systems and their interplays

A dissipative system is one that processes energy and matter in a self-perpetuating, more or less long-lasting exergy-consuming process. In order to function as a unit, a system must have a rather well-defined boundary through which energy and matter flows in and out in a relatively regular way.

A system may be composed of coordinated subsystems. Similarly a group of systems which interact relatively strongly mutually and which are relatively independent of other systems (or depend on other systems in a relatively simple and predictable way) can be considered to form a supersystem.

A few examples:

Cells form organisms. Indiviual persons make up social groups. Together with their land and material property they form communities and societies.

Information is needed for the control and/or coordination of subsystems making up a larger system as well as for adaptation to - or even control of - the environment. Therefore we shall consider systems processing not only matter and energy but also information.

At the boundary of a system there is often a shell[33] protecting from disturbances from the outside and from losses to the outside. The skin of an animal, the walls and roof of a house, and the border protection of a country are examples of such shells.

Between different systems of a similar kind within a supersystem there are networks[33] that channel the flows of energy, matter (different materials), and information. In an animal the blood vessels and the nervous system may serve as examples. In a society there are for instance the transportation network and the telecommunication network.

Clearly shells and networks in a society are closely tied to its exergy consumption: Exergy leaks through the walls and the roof of a house; the transportation system costs a lot of exergy to operate*); a lot of exergy goes into the production of shell and network structures.34)

Exergy goes into the biosphere through the photosynthesis of the green plants (producers) along food chains or foodwebs through higher trophic levels (consumers).At each level exergy is consumed, finally by the decomposers that again mineralize the organic material and make it available for plants.35) Some matter may be stored for a long time in biomass like trees or in fossile layers. On the whole, however, the matter takes part in circular flows, the cycles of water, of carbon, of oxygen, nitrogen, sulphur etc.35)

These cycles extend outside the living world and form part of the geophysical-geochemical system of the earth. Concepts similar to those used in ecology may be used also to describe these systems, their intakes, conversions, and outputs of matter and exergy, and their exergy budgets.

Also for describing exergy flows and matter flows through a society or an economy and the exergy consumption in various subsystems ecological concepts may be useful. The same may be true of information flows through information processing systems as described by Blackburn36) in a paper on the ecology of knowledge.

The relation between exergy and information may be quite complex in practical life. A broken or worn out tool may have lost only little information or exergy. However to replace the information loss by repairing the tool may be costly in terms of exergy. To replace an irrepairable tool may be even more costly.

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*) The nervous system does not!

Natural resources and societal resources can be stocks or flows.[14] Stocks like a forest or a factory that channel useful flows may be called funds[14] or living stocks. The atmosphere, the hydrosphere and the biosphere are funds channelling solar exergy into forms accessible to the human society. Deposits or dead stocks are stocks which do not channel continuous flows but which may give rise to resource (exergy) or information flows over a limited time, like deposits of oil, coal or metals. Table V introduces this terminology.[37]

Stocks and flows of natural resources and societal resources should be accounted for in terms of exergy and information. Such accounting should be done in geophysics, in biology and in economics. Work of this kind has already started in the economic field with the accounting known as energy analysis.[13, 38]

When describing the resource use of a society it is important to work at the right system level. Historically population pressure of man on resources has been of importance and it still is.[39] However more and more a system pressure[40] on the resources is dominating. Production systems, distribution systems (coupled to wasteful consumption practices) and military systems, inadequate - on the global scale - to fulfil basic human needs, live their own life, develop their own impersonal needs, and consume increasing amounts of exergy. Such supersystems are served by people rather than run by people. "Servants" may be of different ranks and power (influence) and there is a positive correlation between rank and personal benefits, material or social. It is of importance to study the functioning of such supersystems, their parasitic relations to humans and to nature, and the societal forces that keep them going - and the forces that act against them.[41]

Within a total system under study certain components with a similar functioning may be lumped together (aggregated) into "compartments".[42] The flows of exergy, matter and information between the compartments of the system are essential for descri-

Table V. Stocks and flows of natural and societal resources

STOCKS

	Natural resources	Societal resources	
		Physical	Human
Dead stocks (Stored resources)	Deposits, e.g. coal, iron ore,..	Stocks of entracted raw materials. Stored products	
Living stocks (Funds)	The geophysical system The biosphere		Population
The economic system of production	Land	Fixed capital	Labour force

FLOWS

	Natural resources	Societal resources	
		Physical	Human
In flows	Solar radiation	Flows extracted from natural cycles - from deposits	Human labour
Out flows	Heat radiation from the earth	Flows returned to natural cycles Waste depositing Flows to natural cycles of new or rare compounds	Human consumption
Circulating flows	The earth's material cycles	Material cycles in society	

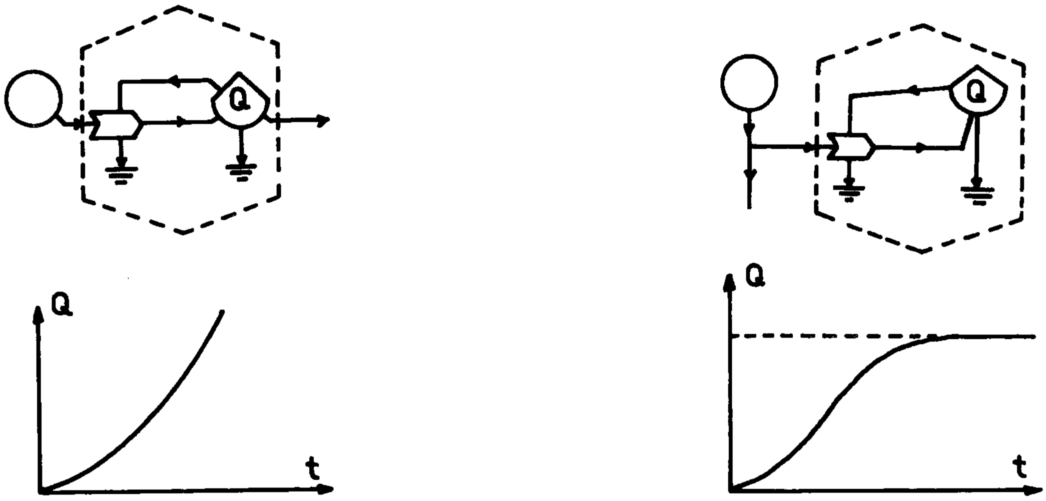
bing the functioning of the system. Some flows may be essential to trigger other flows. If it is possible to construct a realistic model for how some flows steer others in the system, then the system may be simulated by a computer. Aggregation and model building can be done at different system levels. An essential mechanism for the functioning of the whole system may be hidden at one level but clearly seen at another level.

One way to visualize compartments and flows between them in the stationary case is to use a diagram technique like that of H T Odum[42)]. A mathematical description of the same thing can be done for N compartments using N x N flow matrices, $\underline{F}_{ij}$ (the flow from the j th compartment reaching the i th compartment). The flow $\underline{F}_{ij}$ is also a vector,

$$\underline{F}_{ij} = ((F_{ij})_1, \ldots, (F_{ij})_n) \qquad (139)$$

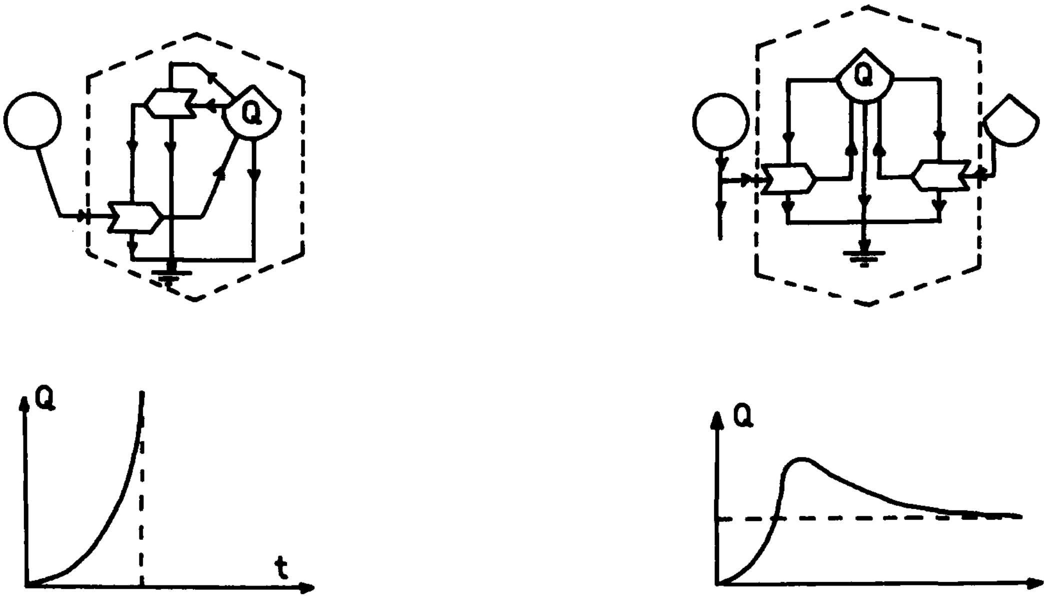
where each of the n vector components describes a certain flow: exergy (possibly decomposed into different forms like heat, chemical exergy, and electricity) and various material flows.

In Fig. 15 we show some standard cases[43)] of a system using a (one-dimensional) resource for its own growth. In the first four cases (a - d) the system is alone, using the resource. In the last two cases (e-f) two systems are competing. In d one of the competitors has a privileged position but functions so that a certain fraction is always left for the other system downstream. Then they stabilize at different non-zero levels. In f the competitors are placed in the same position but nothing prevents one of the systems from taking all that can be taken of the resource. In this case only the fittest system survives.



a) Feedback accelerated growth from source with no limit on flow

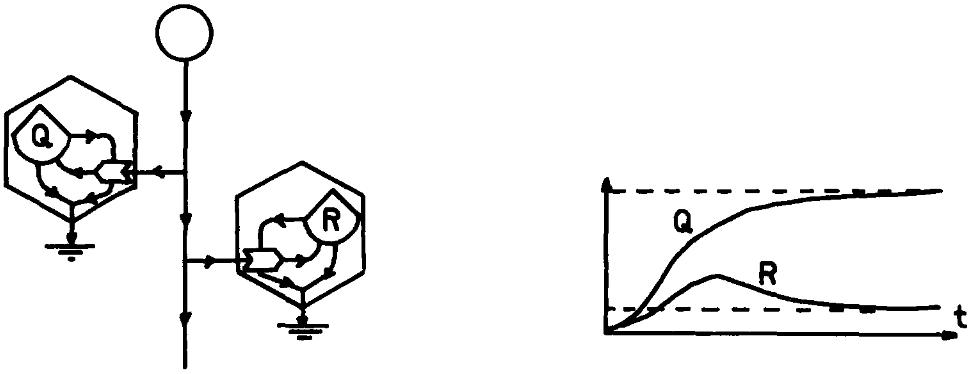
b) Feedback accelerated growth from source with limited flow



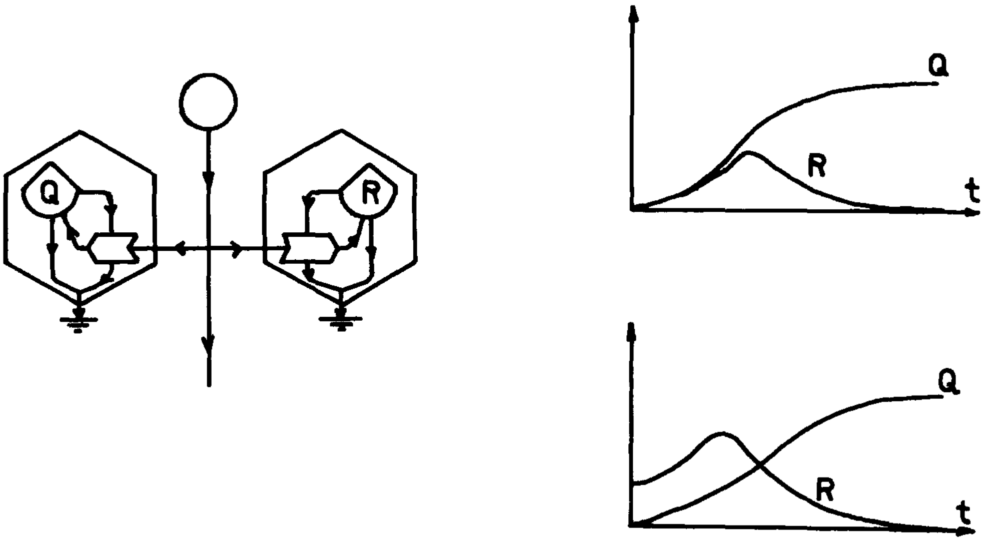
c) Superaccelerated growth from source with no limit on growth

d) Feedback accelerated growth from storage and source with limited flow

Fig. 15 a-d



e) Two competing systems where one of competitors has a privileged position but functions so that a certain fraction is always left for the other system downstream



f) Two competing systems where nothing prevents the most fitted system from taking all that can be taken of the resource

Symbols:

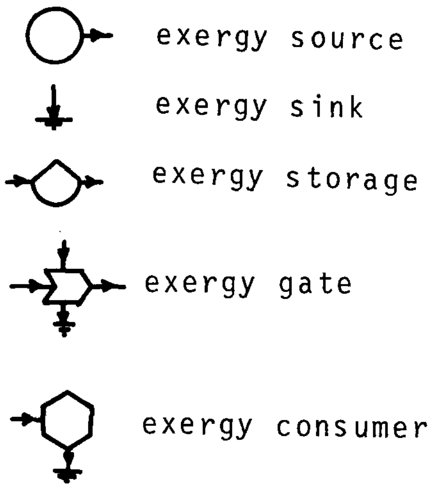


Fig. 15 e and f

It is also necessary to take into account the exergy consumption within the compartments and along the flows. Since exergy appears in several if not all of the n components it is convenient to describe exergy consumption by a sink (negative source) vector which may also include losses of matter. The sink vector for the compartments is a column vector $\underline{G}_j$. The corresponding vector for the flows is a matrix $\underline{H}_{ij}$. We also include sources $\underline{S}_i$. The combined equation for exergy consumption and conservation of matter is then (Fig. 16)$^{x)}$

$$\underline{\underline{M}}^{(i)}\left(\sum_j \underline{F}_{ij}+\underline{S}_i\right)-\underline{G}_i-\sum_j\left(\underline{F}_{ji}+\underline{H}_{ji}\right)=\underline{O}_i \qquad (140)$$

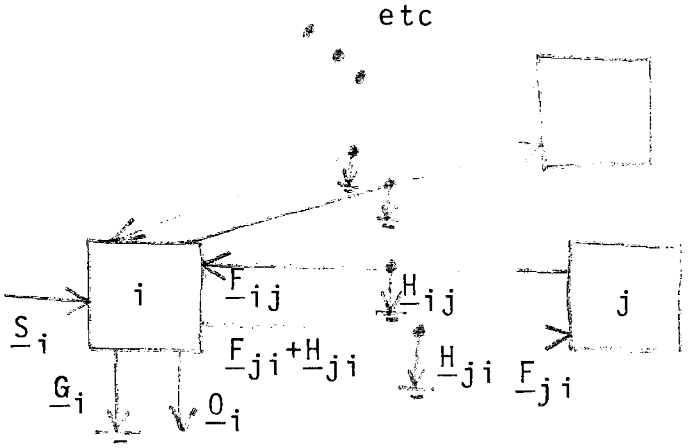


Fig. 16 Exergy consumtion and matter conservation. (Only flows connected to compartment i are indicated.)

where O_i are outputs and where the (nxn) transformation matrix $\underline{\underline{M}}^{(i)}$ describes how the inflows $\underline{F}_{ij}$ into compartment i are transformed into outputs (for instance through chemical reactions).

Let us assume that the output vector

$$\underline{O}=\sum_i \underline{O}_i \qquad (141)$$

---

x) A more complete model would also include the stocks contained in the various compartments.

may be considered to determine the whole system in the neighbourhood (in the n-dimensional $\underline{O}$-space) of a stationary point $\underline{O}^{(o)}$. We may define local coordinates in this neighbourhood

$$\underline{\xi} = \underline{O} - \underline{O}^{(o)} \tag{142}$$

The equation of motion may be written

$$\frac{d\underline{\xi}}{dt} = \underline{C}(\underline{\xi}) \tag{143}$$

That the system is stationary at $\underline{O}=\underline{O}^{(o)}$ means that

$$\underline{C}(0) = 0 \tag{144}$$

and in the neighourhood of $\underline{\xi}=0$ we may take the linear term of an expansion

$$C_{\alpha}(\underline{\xi}) = \sum_{\beta} C_{\alpha\beta}\, \xi_{\beta} \tag{145}$$

where $C_{\alpha\beta}$ is the so-called community matrix.44)

The system is stable if all the eigenvalues of the community matrix have negative real parts. Then the community matrix is said to be qualitatively stable. The necessary and sufficient conditions for this are44)

$$\begin{cases} C_{\alpha\alpha} \leq 0, & \text{all } \alpha \\ C_{\alpha\alpha} < 0, & \text{some } \alpha \\ C_{\alpha\beta} C_{\beta\alpha} \leq 0, & \text{all } \alpha \neq \beta \\ C_{\alpha\beta} C_{\beta\gamma} \cdots C_{\varepsilon\phi} C_{\phi\alpha} = 0, & \text{for any sequence of three or more different indices} \\ \det(C_{\alpha\beta}) \neq 0 \end{cases} \tag{146}$$

13 Acknowledgements

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