Chapter 5

The laws of thermodynamics: entropy, free energy, information and complexity

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Abstract

The laws of thermodynamics have a universality of relevance; they encompass widely diverse fields of study that include biology. Moreover the concept of information-based entropy connects energy with complexity. The latter is of considerable current interest in science in general. In the companion chapter in Volume 1 of this series the laws of thermodynamics are introduced, and applied to parallel considerations of energy in engineering and biology. Here the second law and entropy are addressed more fully, focusing on the above issues. The thermodynamic property free energy/exergy is fully explained in the context of examples in science, engineering and biology. Free energy, expressing the amount of energy which is usefully available to an organism, is seen to be a key concept in biology. It appears throughout the chapter. A careful study is also made of the information-oriented ‘Shannon entropy’ concept. It is seen that Shannon information may be more correctly interpreted as ‘complexity’ rather than ‘entropy’. We find that Darwinian evolution is now being viewed as part of a general thermodynamics-based cosmic process. The history of the universe since the Big Bang, the evolution of the biosphere in general and of biological species in particular are all subject to the operation of the second law of thermodynamics. Our conclusion is that, in contrast to the rather poor 19th century relationship between thermodynamics and biology, a mainstream reconciliation of the two disciplines is now emerging.

1 Introduction

1.1 General

The Industrial Revolution in Britain at the end of the 18th century stemmed from the invention of the steam engine by Watt. The theory of this engine was elaborated half a century later by the
French scientist Sadi Carnot who was the first to formulate the second law of thermodynamics. From then on thermodynamics became a new philosophy in physics, developing over a parallel timescale to that of evolutionary biology.

In the science of the Renaissance time did not feature in the description of phenomena, the laws of physics having a reversible character. Notably Galileo and Newton did not consider the direction of transformations: their mechanistic world was governed by simple reversible principles. Thermodynamics was to change this. While physics at the time of Newton was concerned with optics, mechanics and electrostatics, at the end of the 18th and through the 19th centuries (i.e. because of the Industrial Revolution) the theory of heat became equally important. Relationships between thermal and mechanical forms of energy began to attract attention, which stimulated the development of thermodynamics. Scientists soon came to the conclusion that while mechanical energy can easily be converted into heat, thermal energy cannot be wholly converted into mechanical energy. Carnot (1824) dealing with the maximisation of conversion of thermal into mechanical energy found that there is a limit to the process of energy conversion. This limit was eventually expressed by Clausius’s formulation of the second law of thermodynamics. The second law provides a constraint on the use of energy, in that although the total energy does not change, its ability to generate work depends on a special feature of the energy. This feature was termed ‘entropy’ by Clausius and defined as the quotient of ‘heat’ and ‘temperature on the absolute scale’. Further, Clausius postulated that the entropy of any isolated system would as a general rule increase and entropy began to be interpreted as disorder. Finally, the realisation that this also would hold for the universe gave a direction of change for the universe. The second law introduced the importance of time into science [1].

Unlike, say, energy entropy is not an immediately understandable scientific variable. This is partly because it has a number of different aspects. There is the original phenomenological or thermal meaning, then the microscopic or statistical meaning from the work of Boltzmann, and most recently the information meaning, related to Shannon’s communication theory. Many scientists think that these three formulations of entropy are equivalent, although the third form does require rather careful understanding. This opens new possibilities for the application of thermodynamics to such diverse fields as medicine, history and social processes [2].

Classical physics and chemistry deal with isolated and closed systems. Recently, however, science and engineering have become more interested in open systems [1,2]. Apart from engineering applications, open systems are common in biology, medicine, economics, sociology and history. With closed systems their entropy can increase and the systems finally reach a state of equilibrium. Open systems, on the other hand, and living organisms in particular, can exist in a far-from-equilibrium steady state under conditions of a continuous import of matter and energy from the surroundings [3, 4]. At this point we stress that these latter are accepted characteristics of living systems, stemming from the description given by Schrödinger in his What is Life? lectures of 1944. ‘The living organism . . . keeps alive . . . by continually drawing from its environment negative entropy’ ([5], p. 71; [6], p. 88). The Nobel prize-winning thermodynamicist Ilya Prigogine described [5] as ‘a beautiful book’ ([7] p. 242), and Schrödinger’s exposition not only inspired him but also the mathematician Roger Penrose ([6], p. xx). Prigogine uses the expression ‘a flow of free energy carried by matter . . . which “feeds” the living system’ ([7], p. 239), while Penrose goes right back to the ‘Sun’s role as a source of low entropy (or ‘negative entropy’, in Schrödinger’s terminology)’ ([6], p. xx). This thermodynamic necessity for the existence of living organisms carries forward into current mainstream biology. In the standard US text Life, W. Purves et al. [8] explain: ‘Free energy is what cells require for . . . cell growth, cell division and the maintenance of cell health’ ([8], p. 97) and context).
A final, more general point, is that systems far-from-equilibrium can undergo evolution to a new level of order. This has application to the behaviour of complex systems.

In this chapter, thermodynamics is applied to examples in physics (magnetism), in engineering (exergy analysis of a nuclear power system) and to biology (glycolysis in cells). While the first two examples are at the level of understanding of the latter years of undergraduate courses, there is sufficient background in [9] and in this chapter to follow these through. The identity of thermal and statistical entropy is then demonstrated and the role of entropy in contemporary studies surveyed. The validity of ‘Shannon entropy’ is carefully addressed together with the quantitative definitions of information and complexity. The core of the whole biological/thermodynamic synthesis is dealt with, for the cosmos, for the biosphere and then for species.

Overall, we have sought to elucidate our theme from a variety of angles. We conclude with a discussion of some of the consequences of our overall approach, and by stressing that a mainstream reconciliation, if not orthodoxy, of thermodynamics and biology is clearly developing.

1.2 Closed, open and isolated systems

Thermodynamics is the only science that deals with inherent directionality. Jeffrey Wicken [10], p. 65

... he became fascinated by the apparent contradiction... suggested by the second law of thermodynamics and Darwinian evolution... to more complex and ordered structures.


In this chapter, we consider three kinds of systems. A closed system is of fixed mass, with possible heat and work transfers across its boundary. An open system has, in addition to possible heat and work, mass flows across its boundary. An isolated system is a closed system with no heat transfer. Classical physics and chemistry deal with closed systems in a state of equilibrium. A system is in equilibrium if its parameters are uniform in space. Equilibrium processes are ideal processes which do not occur in nature. When a system changes from one state to another, its equilibrium is lost. In practice though, it is sufficient that the time needed for a state to reach equilibrium is smaller than the time of change from one state to another. In classical terms, the relaxation time is shorter than the duration of the phenomenon. This is a key underlying assumption of ‘equilibrium thermodynamics’ which, while idealised, is a satisfactory description of a whole range of engineering processes.

An isolated system, initially in a non-equilibrium state, will always tend towards equilibrium. Such a process is called spontaneous. Now reversal of a spontaneous process is impossible. This is the most general formulation of the second law of thermodynamics and expresses Wicken’s ‘inherent directionality’ of change in natural processes. It is written in mathematical form using the entropy $S$, where changes for an isolated system are always non-decreasing:

$$dS_{\text{isol}} \geq 0. \quad (1)$$

As we have noted, the concept of entropy was formulated by Clausius in 1850. It is defined in the following way:

$$dS_{\text{def}} = \frac{dQ^\circ}{T}. \quad (2)$$
where \( dQ \), represents the total heat transfer to or from the system and \( T \), is the absolute temperature of the system.

In Section 1.1 we pointed out that open systems are of increasing interest in science and engineering and are also found in biology, medicine, economics, sociology and history. It is the essential differences between closed/isolated and open systems which removes the ‘apparent contradiction’ which fascinated Prigogine. Living organisms are open systems.

In an open system, as formulated by Prigogine:

\[
dS = d_eS + d_iS,
\]

where \( d_eS \) denotes the change of entropy due to the influx of mass from the surroundings, \( d_eS \) is the entropy rise due to irreversibility of changes taking place in the system; \( d_eS \) is always positive whereas \( d_iS \) can either be positive or negative. \( dS \), then, can be negative, i.e. the entropy of the system reduces, such a process being frequently referred to as ‘negentropic’. In living organisms this ‘negentropic’ effect is not inconsistent with the second law of thermodynamics.

1.3 Complex systems

The historical development of thermodynamics focused on the production of mechanical work. This resulted from a change of shape (expansion) of a system, usually comprising a fluid substance such as steam/water or gas. However, thermodynamics is much more generally applicable, and can involve systems such as magnetic substances, surface membranes and elastic (solid) bodies. Correspondingly, thermodynamic work is widely defined to include that caused, for example, by electrical, rotational, chemical and surface tension forces. Systems which can perform a number of different types of work are formally defined in the context of thermodynamics as ‘complex systems’, involving what are referred to as ‘complex substances’. However, these expressions should not be confused with the rather similar expression ‘complex structures’ as used to describe biological systems. The latter really arises from more general complexity studies, not thermodynamics. Finally, our use of the word complexity will refer to the quantifiable Shannon information measure of structured systems in general.

2 Application of classical thermodynamics to physics

2.1 The calculation of mechanical work

One of the first applications of the closed system concept in thermodynamics is its key application to mechanical work. Such work is done when a system increases its volume (see equation (1) in [9]), so that:

\[
dW = pdV.
\]

Most frequently this involves a compressible substance, such as a gas. For the equation to be integrated, it is essential to know the relationship between \( p \) and \( V \). In fact, for a gas, the absolute temperature \( T \) is also involved. To calculate the work for a given process, the relationship may be expressed as:

1. model equations, such as ‘perfect gas’ and ‘real gas’ equations;
2. thermodynamic graphs, such as the old engineering ‘steam charts’;
3. thermodynamic tables, such as the engineering ‘steam tables’ or ‘property tables’.
In this treatment, we define the perfect gas and give an example of a real gas, the Van der Waals’ gas.

### 2.1.1 The perfect gas

The thermal state equation for a perfect gas has the form:

\[ pV = RT \quad \text{or} \quad pV = mRT, \]  \hspace{1cm} (4)

and is sometimes called the Clapeyron equation.

The experiment of Joule concerning expansion of gases to a vacuum proved that the change of the gas volume does not change the energy of the internal gas.

\[ \left( \frac{\partial u}{\partial V} \right)_T = 0. \]  \hspace{1cm} (5)

That is, for a constant volume there is no work transfer, and the heat transfer \( dq \) by the first law of thermodynamics is equal to \( du \).

\[ dq = du = \left( \frac{\partial u}{\partial T} \right)_V dT = f(T) dT. \]  \hspace{1cm} (6)

It follows from the above that

\[ du = c_v dT, \]  \hspace{1cm} (7a)

which means that the internal energy depends only on the temperature. The above equation is called the **caloric equation for a perfect gas**. For a compressible substance in general \( u \) is given by

\[ u = u(T, v), \]  \hspace{1cm} (7b)

and this becomes \( u = u(T) \) for the perfect gas.

### 2.1.2 A real gas

Based on the molecular structure of matter, Van der Waals suggested a modification of the state equation for a perfect gas which takes into account the effect of molecular attraction in the pressure term and effect of molecular volume in the specific volume term:

\[ \left( p + \frac{a}{v^2} \right) (v - b) = RT. \]  \hspace{1cm} (8)

This model of a real gas is only qualitatively good, and other \( p, V, T \) relationships may be specified. As mentioned above, for engineering calculations thermodynamic graphs and tables are used (now, most commonly, the latter) near the phase-change boundaries.

What eqn (4) implies is that the thermodynamic state of a substance may be defined by the choice of two properties. This is an expression of the so-called ‘two-property’ rule. It is termed a rule, rather than a law, because under certain conditions (e.g. mixed-phase) some of the properties are not independent.

### 2.2 The simple magnetic substance

Classical equilibrium thermodynamics is relevant to the entire physical world. The above initial example demonstrates how, in order to calculate thermodynamic behaviour, the primary properties of pressure, volume and temperature are related for compressible substances like gases.
A further example, the simple magnetic substance, illustrates how thermodynamics can provide a detailed description of what may be subtle and intricate property behaviour for solids.

For such a substance, it follows from the above two-property rule that by choosing two independent intensive parameters, we may define the state. Using the absolute temperature $T$ and the magnetic field $H$, and starting from similar premises as for compressible substances (say the perfect gas) the thermal state equation can be written in the form:

$$ M = M(T, H), \quad (9) $$

where $M$ is the magnetic moment. This plays the same role for magnetic substances as the volume for compressible substances. The magnetic field $H$, parallel to pressure, gives the mechanical work in a magnetic field as:

$$ dW = -\mu_0 VdM = BVdM, \quad (10) $$

where $\mu_0$ denotes the magnetic permeability and $B = \mu_0 H$ is the magnetic induction.

The caloric equation of state that describes the internal energy can have one of the following forms:

$$ u = u(T, M), $$
$$ u = u(T, H), $$
$$ u = u(M, H), $$

the first form being analogous to

$$ u = u(T, V), $$

for compressible substances in general (equation preceding (7b)).

For magnetic systems we can also define:

- **Magnetic enthalpy**
  $$ H_M = U - \mu_0 VH $$

- **Gibbs function**
  $$ G_M = H_M -TdS = U - \mu_0 VH - TdS = \varphi $$

- **Specific heat at constant magnetic field** $H$ (in analogy to $c_p$)
  $$ c_H = \left( \frac{\partial h}{\partial T} \right)_H $$

and the relation between $c_H$ and $c_M$, where $c_M$ is analogous to $c_V$ (the specific heat of a gas at constant volume):

$$ c_H - c_M = \frac{T\mu_0 V (\partial M / \partial T)^2_H}{(\partial M / \partial H)_T}. \quad (15) $$

One can also obtain Maxwell relations for magnetic systems.

The magnetic moment $M$ is related to the magnetic field $H$

$$ M = \chi H. \quad (16) $$
If $\chi < 0$, then the substances are called \textit{diamagnetic}. They attenuate the magnetic field. Examples of such substances are mercury, silver, copper, or gold. If $\chi > 0$, the substances are called \textit{paramagnetic}. For these substances $B > H$, however $\chi$ does not depend on $H$. Examples are Curie magnetics for which $\chi = A/T$, where $A$ is a constant. If $\chi < 0$ and $\chi$ strongly depends on the magnetic field, then the substances are called \textit{ferromagnetic}. Among ferromagnetic substances are iron, nickel and cobalt.

The magnetic system undergoes changes in structure (phase changes). It appears in two phases: \textit{conductive (paramagnetic)} and \textit{superconductive (ferromagnetic)}. Systems that change from normally conductive to superconductive states are called superconductors. The transition point is called the Curie point. Above the Curie point, the ferromagnetic substance behaves as paramagnetic. For iron, the Curie point is 765$^\circ$C. For magnetic systems, the Curie magnetic can be considered analogous to a perfect gas, as its state equation is expressed by a simple analytical relation:

\[
M = c \frac{H}{T} \quad \text{where} \quad \frac{H}{T} = f(M).
\] (17)

Examples of Curie magnetics can be paramagnetic salts at not too low temperatures and not too high magnetic fields. It can be proved that in this case the internal energy is a function of temperature only.

The temperature does not depend on $M$ for $U = \text{const.}$, which means that $U = U(T)$ for substances for which $H/T = f(M)$. For the Curie magnetic the following relation holds:

\[
du = c_M(T) dT.
\] (18)

For a paramagnetic substance $c_H > c_M$, for diamagnetic $c_H - c_M \approx 0$.

Adiabatic demagnetisation of paramagnetics leads to a decrease in their temperature. This effect is especially strong at low temperatures. Using this approach, temperatures of the order of 0.001$^\circ$C can be achieved.

### 2.3 Complex substances

Complex substances are substances which are subject to more than one type of reversible work. Examples are systems exchanging mass within the same substance and at the same time performing volume work. There are two types of such systems: those undergoing phase changes (physical reactions) and those with chemical reactions. Systems within a field of external forces, such as an electric or magnetic field and those which are at the same time subject to mechanical loads, form a class of complex substances. A number of thermal effects, important from the point of view of applications as well as interesting in terms of cognitive values, occur in these systems. \textit{Pyroelectric} or \textit{pyromagnetic} effects appear in electric or magnetic fields. Among these effects are electrocaloric or magnetocaloric effects that accompany adiabatic processes. In systems subject to mechanical loads, thermoelastic effects occur, whereas in electric or magnetic systems subject to mechanical loads additional effects take place resulting from coupling of the phenomena, the so-called piezoelectric or piezomagnetic effects.

Again, we are using the expression ‘complex substances’ as a whole in a manner similar to ‘complex systems’. 
2.4 Discussion

In this section we have shown how, using methods of classical thermodynamics, the behaviour of typical gases may be described, and an entire mathematical model constructed for magnetic substances. This model incorporates the properties and behaviour of the different classes diamagnetic, paramagnetic and ferromagnetic. It serves to demonstrate how comprehensively thermodynamics applies in the physical world.

3 Application of laws of thermodynamics in engineering

3.1 Introduction

We turn from physics to engineering and emphasise that the laws of thermodynamics enable a range of engineering problems to be addressed.

Now classical thermodynamics does not make use of a co-ordinate system as it deals with equilibrium systems where intensive parameters (such as temperature field, pressure field and concentration field) are uniform in the whole volume.

An important element of thermodynamic analysis is the choice of the system. The classical system is a closed system – connected with a constant mass and same number of molecules. In engineering thermodynamics the concept of the closed system is extended to that of the open system. In the case of the closed system, the application of mass conservation is redundant. In the case of the open system, the conservation of mass and momentum provides complementary information about the behaviour of the system.

3.2 Energy and exergy analysis: the concept of maximum work

Here the level of understanding is that of the final year of an engineering degree course. We have sought to give sufficient background material, here and in [9], to enable an understanding of exergy to be gained, from the following.

An energy conversion chain is accomplished in power stations: from chemical energy to heat to mechanical energy to electrical energy. The efficiency of individual processes is the ratio of the exit energy of the desired type to the energy supplied at the inlet. The efficiency depends on physical and chemical laws governing the processes of conversion. Increasing the efficiency of the process can be achieved by decreasing the amount of energy supplied at the inlet, increasing the energy output at the exit, or a combination of both these methods.

In the companion chapter of the authors in Volume 1 of this Series [9] a description is given of the application of thermodynamics to the generation of power through, especially, fossil fuels. The individual components of a power station (e.g. boiler, steam turbine) are open systems using flow processes. However, for the operation as a whole the H2O working fluid acts as a closed system, and therefore as a heat engine. (The latter is defined as a system operating continuously over a cycle, exchanging heat with thermal reservoirs and producing work.)

The maximum possible theoretical thermal efficiency is provided by the Carnot cycle. However, a simple more practical adaptation results in the Rankine cycle. This, together with superheat and reheat enhancements, provides a theoretical heat engine model for analysis of fossil fuel central electricity generation steam cycles (again see [9] and the typical undergraduate text by Rogers and Mayhew [11]). For the sake of completeness we define our ideal heat engine as follows.
In consistency with the second law of thermodynamics, no heat engine can have an efficiency higher than that of the reversible Carnot cycle. In turn, the first law of thermodynamics implies that the heat input to the cycle, i.e. the difference between the supplied heat and the heat rejected from the cycle, is equal to the cycle work. The efficiency of the Carnot cycle for constant temperatures of the upper source $T_2$ and surroundings $T_1$ is equal to:

$$\eta_c = 1 - \frac{T_1}{T_2}. \quad (19)$$

Apart from the Rankine cycle, a number of other heat engine cycles have been invented since the time of Carnot, some of which form a modification of the ideal Carnot cycle but are not easy to implement in practice. Two, the Stirling and Ericsson cycles ([11], pp. 270–272) have the same theoretical efficiency as the Carnot cycle, but even ideal versions of the others have a lesser maximum.

Apart from the overall cycle, the engineer is interested in the individual flow processes making up the cycle, reflecting the real processes taking place in thermal machinery. Determination of the efficiency of the machine where the energy conversion takes place requires application not only of the first but also the second law of thermodynamics, as the conversion of any type of energy always leads to a fraction of it being changed into heat, which as a consequence gives rise to an entropy change of the system.

For an open system, for which heat $Q$ is both supplied and carried away, the first law of thermodynamics for steady states has the form for work output $W$:

$$W = Q_{\text{in}} - Q_{\text{out}} + \dot{m} (h_{\text{in}} - h_{\text{out}}), \quad (20)$$

noting that $\dot{m}_{\text{in}} = \dot{m}_{\text{out}} = \dot{m}$ (steady state) and $h$ is the enthalpy.

The second law of thermodynamics related to the surroundings can be written in the form:

$$\dot{S} = \frac{dS}{dt} = \frac{Q_{\text{out}}}{T_{\text{ref}}} - \frac{Q_{\text{in}}}{T} + \dot{m} (s_{\text{out}} - s_{\text{in}}) \geq 0, \quad (21)$$

$$ST_{\text{ref}} = Q_{\text{in}} \left(1 - \frac{T_{\text{ref}}}{T}\right) + \dot{m} [(h_{\text{in}} - h_{\text{out}}) - T_{\text{ref}} (s_{\text{in}} - s_{\text{out}})] - W \geq 0. \quad (22)$$

The following equation for the maximum work of the system can be derived from eqn (22):

$$W_{\text{max}} = Q_{\text{in}} \left(1 - \frac{T_{\text{ref}}}{T}\right) + \dot{m} [(h_{\text{in}} - h_{\text{out}}) - T_{\text{ref}} (s_{\text{in}} - s_{\text{out}})]. \quad (23)$$

Now the ability of a system to perform work may be regarded as a sort of ‘quality’ of its behaviour, where the reference level for this ability is the surroundings. At these conditions the work output is zero.

The above quantitative measure, represented by eqn (23) is termed the exergy, and substantial contributions to its recognition and application have been made by Szargut in Polish [12, 13] and by Kotas in English [14].

3.3 Theoretical aspects of exergy

Now the first term in eqn (23) describes the increase of exergy of the heat source, whereas the second term expresses the change of exergy of the working fluid of the system.
For a closed system ($m = 0$), $W_{\text{max}}$ is equal to:

$$W_{\text{max}} = Q_{\text{in}} \left(1 - \frac{T_{\text{ref}}}{T}\right),$$  \hspace{1cm} (24)

which is the same as the work obtained in the Carnot cycle, since $\eta_c = 1 - T_{\text{ref}}/T$.

If in a system, heat is converted to work, then the efficiency of this process (defined by using the first law of thermodynamics) has the form:

$$\eta^I = \frac{W}{Q_{\text{in}} + mh_{\text{in}}}. \hspace{1cm} (25)$$

For a closed system, i.e. when $m = 0$, the efficiency is equal to:

$$\eta^I = \frac{W}{Q_{\text{in}}}, \hspace{1cm} (26)$$

where

$$W = Q_{\text{in}} - Q_{\text{out}}.$$

Another definition of the efficiency – exergy efficiency – that takes into account the energy quality can be derived from the second law of thermodynamics. In this approach, entropy changes – i.e. the irreversibility of the process due to which the work $W$ is obtained instead of $W_{\text{max}}$ are taken into account. The exergy efficiency found in this way is:

$$\eta^{II} = \frac{W}{W_{\text{max}}}, \hspace{1cm} (27)$$

where $W$ is described by eqn (20) and $W_{\text{max}}$ by eqn (23). The difference

$$W_{\text{max}} - W = S T_{\text{ref}} = I$$  \hspace{1cm} (28)

is a loss of work $I$ due to irreversibility of the process. In the case of a closed system $m = 0$, eqn (27) takes the form:

$$\eta^{II} = \frac{Q_{\text{in}} - Q_{\text{out}}}{Q(1 - T_{\text{ref}}/T)} = \frac{\eta^I}{\eta_c}, \hspace{1cm} (29)$$

where $\eta_c$ is the efficiency of the Carnot cycle – the maximum efficiency that can be reached.

Energy analyses of engineering processes based on the first law of thermodynamics and overall analyses based on the second law of thermodynamics enable the determination of energy losses and the evaluation of the maximum possible work which may be obtained from the system. Such analyses can lead to improvements in engineering processes. In fact, because exergy can be regarded as representing the (exploitable) economic value of an energy source, it can be used for the evaluation of the natural environment itself [12].

### 3.4 Exergy and Gibbs free energy – an engineering/biology identity

In eqn (23) the second term – the change of exergy of the working fluid – may be re-expressed as:

$$W_{\text{max}} = \dot{m} \left[\Delta h - T_{\text{ref}} \Delta s\right] = G_{\text{ref}}, \hspace{1cm} (30)$$

where the Gibbs function $G_{\text{ref}}$ is defined by eqn (13).
In [9] Mikielewicz et al. pointed out that \( G \), too, represents maximum available work, and the above shows that exergy and Gibbs function are essentially identical, if \( T = T_{\text{ref}} \).

Now it is the ‘Gibbs free energy’ or just ‘free energy’ that is the standard descriptor for biological energy processes ([8], 97 ff. – compare with the earlier edition [15] (p. 117); [7], p. 239; [10], p. 36; [16], p. 18 or [17], p. 37). So, here too, via thermodynamics, engineering and biology are intimately connected.

### 3.5 The application of exergy – an example

As part of a series of final-year undergraduate projects supervised by Collins [18] exergy analyses were carried out for two (MAGNOX and AGR) UK nuclear power reactor systems used for electricity generation. Now in using nuclear power as an example, it is important to note that at the time of writing this chapter the first political signs are evident that in the UK at least this energy source may need renewing [19]. Under the subheading ‘Timms hints at fresh nuclear builds’, the Energy Minister is reported to have said ‘In the future we may realize that there is a place for nuclear power and new nuclear builds’.

Based on the work of Kotas [14], and ignoring potential and kinetic energy and chemical reaction effects, the change in exergy between two points is:

\[
E_1 - E_2 = (H_1 - H_2) - T_{\text{ref}}(S_2 - S_1)
\]

or, per unit mass,

\[
e_1 - e_2 = (h_1 - h_2) - T_{\text{ref}}(s_2 - s_1).
\]

In any real (irreversible process) with \( W \) and \( Q \):

\[
E_1 - E_2 = W - Q + I,
\]

where \( I \) is the irreversibility of the process.

What is termed the ‘rational efficiency’ is:

\[
\Psi = 1 - \frac{I}{\sum E_{\text{in}}},
\]

with the efficiency defect \( \delta \):

\[
\delta = 1 - \Psi
\]

and component inefficiencies \( \delta_i \) given by:

\[
\delta_i = \frac{I_i}{\sum E_{\text{in}}} \quad \text{where} \quad \Psi + \sum \delta_i = 1.
\]

Using these parameters, the exergy balance for a plant may be expressed diagrammatically as Grassman and pie chart figures.

The first phase of the UK nuclear programme was based on the Magnox reactor system, with natural uranium as fuel, non-oxidising magnesium as cladding, carbon dioxide as primary coolant and a steam cycle for electricity generation. The plant diagram was simplified to final-year thermodynamics teaching level, and typical temperature and pressure data defined. The plant diagram is shown in Fig. 1, with calculated values of \( h, s \) and \( e \) incorporated into Table 1. From this, an exergy pie chart and Grassman diagram were constructed as in Figs 2 and 3.
Thermodynamically speaking, the main problem with the Magnox system was the low working temperatures. These were associated with the permitted maximum fuel and cladding temperatures and to avoid excessive creep and other problems in the original steel pressure vessels. As a consequence, the heat exchangers, under the ‘burden’ of a low temperature difference, had to be of very high surface area. This component inefficiency dominated the whole cycle (see Fig. 2).
resulting in a low overall thermal efficiency. The subsequent AGR system used enriched uranium fuel and stainless steel cladding, and did not have this drawback.

In general, exergy analyses quantify the various losses in a cycle, giving a focus on where design improvements should most usefully be made.
4 Application of thermodynamics to biology – glycolysis and the tricarboxylic acid (Krebs) cycle

The essential similarity of exergy and (Gibbs) free energy has been noted and is formally analysed by Rogers and Mayhew ([11], pp. 117–125). Our engineering example has not involved chemistry, whereas the free energy analyses for biological cell energy cycles are exclusively chemical in character ([8], chapter 7). By taking glycolysis and the tricarboxylic acid cycle as an example, we are extending the application of thermodynamics to encompass the physical, engineering and biological worlds, and of exergy/Gibbs free energy to both thermal and chemical processes.

Glycolysis is a 10-reaction series of chemical processes in the living cell, whereby the substrate glucose is transformed into pyruvate. It is common to aerobic and anaerobic metabolism, as shown in figure 16 of the companion chapter in Volume 1 of this series [9]. In aerobic metabolism, glycolysis is followed by pyruvate oxidation and the tricarboxylic acid cycle, before entry of reducing potential (arising from oxidative processes in glycolysis and the tricarboxylic acid cycle) into the respiratory chain. Like glycolysis, the tricarboxylic acid cycle is a multi-process series.

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Table 2, using data from [8] and [15] shows the progression of free energy through the complex chemistry. It can be seen that the release of free energy is much greater in the tri-carboxylic acid cycle than in glycolysis.

On comparing Tables 1 and 2 it is apparent that the overall multi-stage character of the thermodynamics processes are of a similar order of magnitude. However, while most biological

<table>
<thead>
<tr>
<th>Process</th>
<th>Stages</th>
<th>Free energy change $\Delta G$ (kcal)</th>
<th>Process change $\Delta G$ (kcal)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glycolysis</td>
<td>Glucose</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Glucose 6-phosphate</td>
<td>+5.4</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Fructose 6-phosphate</td>
<td>+7.9</td>
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<tr>
<td></td>
<td>Fructose 1,6-biphosphate</td>
<td>+11.6</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Dihydroxyacetone phosphate</td>
<td>+15.9</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Glyceraldehyde 3-phosphate</td>
<td>+18.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1,3-Bisphosphoglycerate</td>
<td>−83.6</td>
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</tr>
<tr>
<td></td>
<td>3-Phosphoglycerate</td>
<td>−110.3</td>
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<tr>
<td></td>
<td>2-Phosphoglycerate</td>
<td>−10</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Phosphoenolpyruvate</td>
<td>−109.1</td>
<td>−137.6</td>
</tr>
<tr>
<td></td>
<td>Pyruvate</td>
<td>−137.6</td>
<td>−112.3</td>
</tr>
<tr>
<td></td>
<td>Acetyl CoA</td>
<td>−249.9</td>
<td></td>
</tr>
<tr>
<td>Pyruvate oxidation/</td>
<td>Citrate (citric acid)</td>
<td>−273.4</td>
<td></td>
</tr>
<tr>
<td>Tricarboxylic acid cycle</td>
<td>Isocitrate</td>
<td>−259.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\alpha$-Ketoglutarate</td>
<td>−370.9</td>
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</tr>
<tr>
<td></td>
<td>Succinyl CoA</td>
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<tr>
<td></td>
<td>Succinate</td>
<td>−572.0</td>
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<tr>
<td></td>
<td>Malate</td>
<td>−581.6</td>
<td>−418.8</td>
</tr>
<tr>
<td></td>
<td>Oxaloacetate</td>
<td>−668.7</td>
<td></td>
</tr>
</tbody>
</table>
cells have diameters between 1 and 100 microns (1 \( \mu m = 10^{-6} \) m) ([8], p. 56), the overall site dimension of a Magnox power station is in the kilometre range. Later in the chapter the reasons for this mismatch between engineering and biological ‘power systems’ will be discussed.

5 Equivalence of thermal and statistical entropy

5.1 The role of thermal entropy – a summary

In the preceding sections, thermodynamics has been applied within the physical, engineering and biological worlds. Whether in the form of mathematical relationships, quantitative calculations or measurement data, thermodynamics facilitates a clear understanding of the underlying science. While the first law focuses on the relatively understandable concept of energy, the second law shows that the absolute temperature is a crucial factor in thermodynamic performance. The combination of ‘heat transferred’ and the ‘temperature at which the heat is transferred’ is represented by the (phenomenological or thermal) entropy. So entropy enters, via exergy or Gibbs function, the interpretation of thermodynamic efficiency and maximum available (or ‘free’) energy, whether in a nuclear power system or in a biological cell. Finally, our engineering example has not involved chemistry, whereas the cell energy processes are exclusively chemical in character ([8], Chapter 7). Thermodynamics copes equally well with both, so this contrast demonstrates still further its all-pervasive applicability within the engineering and natural worlds.

5.2 Statistical entropy

The ‘genius’ of thermodynamics includes its ability to address large scale structures (e.g. steam turbines) on the one hand and detailed molecular and property behaviour on the other. For engineering thermodynamics in particular, the system concept (whether closed, open or isolated) means that a ‘black box’ approach is elegantly feasible. By judicious choice of the system boundary, problematic internal components, effects and processes can be virtually ignored, provided, as is usual, equilibrium can be assumed. This is because the first and second laws relate to system boundary transfers such as work and heat, and properties for the system as a whole, say internal energy. As a consequence, this can be a powerful approach when applied to living systems such as Homo sapiens.

At the same time, thermodynamics can be expressed theoretically in terms of, for example, the partial differential Maxwell relations between properties. This has already been apparent here in the treatment above of magnetic substances. Such properties can be related to molecular behaviour.

This macroscopic/microscopic comparison is directly relevant to entropy. In the section above we surveyed the place of thermal entropy in a variety of situations. Boltzmann, however introduced the concept of statistical entropy related to the probability of the microstates of individual molecules comprising a system.

Briefly, this is as follows. Boltzmann treated entropy as a measure of disorder of molecules forming a system:

\[
S = -k \sum_i (p_i \ln p_i),
\]

where \( k \) is the Boltzmann constant equal to \( 1.38 \times 10^{-23} \) having dimensions of entropy. The symbol \( p_i \) denotes the probability of occurrence of a microstate. The equation corresponds to a
single molecule, or more precisely, to each degree of freedom possessing a few microstates. The contribution of all degrees of freedom is summed up for the entropy of the system. The total energy of the degree of freedom is $E = kT$ and acts as a restriction for $p_i$. At low temperatures some degrees of freedom are frozen and do not contribute to energy. At zero temperature on the absolute scale, all degrees of freedom have a probability equal to one or zero, and it is then obtained that $S = 0$, in consistency with the third law of thermodynamics. Distinguishing between the molecular microstate and degree of freedom of the system is important from the point of view of information theory because one can speak about the entropy of individual degrees of freedom.

5.3 Equivalence of thermal and statistical entropy

It is possible to prove the equivalence of thermal and statistical entropy using the example of a perfect gas. Let us consider an irreversible process of expansion of a perfect gas in a vacuum. Due to the fact that the surroundings is a vacuum, the system does not yield work (lack of back-pressure). The system as a whole is isolated, therefore its energy and temperature do not change. For an isothermal process

$$dW = pdV = dQ.$$  

And therefore the entropy change is equal to:

$$dS = \frac{dQ}{T} = \frac{pdV}{T}.$$  

Making use of the state equation for a perfect gas (4), one can obtain

$$dS = R \frac{dV}{V}. \quad (37)$$

Let us consider the same process from the microscopic point of view. The probability of finding a molecule in the initial volume $V_1$ is equal to:

$$pV = \frac{V_1}{V_2}. \quad (38)$$

where $V_2$ is the final volume.

The probability of finding $N$ molecules in the initial volume $V_1$ is still smaller and due to the independence of events is equal to:

$$p_N = \left( \frac{V_1}{V_2} \right)^N. \quad (39)$$

Taking a logarithm from the above equation one can obtain

$$\ln p_N = N \ln p_V = N \ln \frac{V_1}{V_2}. \quad (40)$$

Let us assume that $V_2$ does not significantly differ from $V_1$, i.e. $V_2 = V_1 + dV$. Then

$$\frac{V_1}{V_2} = 1 - \frac{dV}{V}.$$  

Taking a logarithm and expanding into a series, one can get

$$\ln \frac{V_1}{V_2} = \ln \left( 1 - \frac{dV}{V} \right) \approx -\frac{dV}{V}. \quad (41)$$
Then
\[ \ln p_N = -N \frac{dV}{V}. \]  
(42)

Using eqn (37)
\[ dS = -\frac{R}{N} \ln p_N. \]  
(43)

5.4 Consequences

So a relationship between the thermal entropy and the probability of occurrence of a given state of molecules is evident. The consequence is that the entropy statements of the second law of thermodynamics may be reformulated in terms of the probability of occurrence of given states of molecules. Thus an irreversible process now means a process of change from a less to a more probable microscopic state. The (thermal) Planck statement of the second law [9] is: ‘it is impossible to construct a system which will operate in a cycle, extract heat from a reservoir, and do an equivalent amount of work on the surroundings’. Such a device is described as a perpetual motion machine of the second kind (or PMM2). However, the statistical formulation of the second law states that a PMM2 is not impossible but highly unlikely. There is, similarly, little probability of an expanded gas contracting to its initial volume, and even less probability that such a process could be repeated in a cycle.

To summarise, the statistical aspect of entropy requires the subtle re-interpretation of the second law away from absolutism to that of being very highly probable.

6 Role of entropy in contemporary studies

6.1 The different aspects of entropy

Firstly, we extend our comparison of thermal and statistical entropy to include that due to the information theory of Shannon. In brief the three aspects may be distinguished as [20]:

1. Thermal, or phenomenological, as already applied in Sections 2–4.
2. Statistical, after Boltzmann, as explained in Section 5.2.
3. Informatic, related to the information contained in a message, forming part of communication theory.

A number of researchers believe these three formulations are equivalent to each other. The first to reach this conclusion was Brillouin [21] and more recently, Peters [22]. Others, such as Wicken, strongly dispute this equivalence. Typical of his statements is ‘This misapprehension blurs fundamental issues’ ([10], p. 18). In Section 7 the pros and cons of ‘Shannon entropy’ will be reviewed.

6.2 Information theory

This description follows Thoma’s comprehensive, but externally unpublished, study [23]; Shannon’s source material may be found in [24].

According to Shannon, information is the message content of a signal. Each signal takes a certain position in the message and can assume a number of discrete values, each value with a probability \( p_i \), where \( i \) changes from 1 to \( m \) and \( \sum_{i=1}^{m} p_i = 1 \).
The information transported through a given symbol \( i \) is \( \log_2 p_i \). The logarithm with a base 2 is chosen here, as with a 50% probability, it gives the unit information called a bit. The average contribution of symbol \( i \) to information is \( p_i \log_2 p_i \). The message is a sum of all possible pieces of information

\[
H = -K \sum_i p_i \log_2 p_i. \tag{44}
\]

In binary notation, \( m = 2 \) and \( p = p_i \text{ or } p = 1 - p_i \).

In the above equation, the constant \( K \) is usually taken as unity ([10], p. 19) and \( H \) is the Shannon or confusion functional ([23], p. 7). In fact, \( H \) is customarily taken to be entropy, for example, being so used throughout in a biological context by Brooks and Wiley [25].

The transmitted information \( I \) is defined as the difference in the values of \( H \) before and after the communication of a message:

\[
I = -(H_{\text{after}} - H_{\text{before}}). \tag{45}
\]

\( I \), being of opposite sign to \( H \), becomes the widely used term ‘negentropy’.

As an example, assume that the memory of an element contains 1024 responses with equal probability \( p_i = 1/1024 \) for each response before the information. Then, according to the above formula, the information before receipt is equal to 10. After receipt of the information only one signal is certain, the other signals having a zero probability. The obtained information contains 10 bits, therefore. Now as Wicken notes ([10], p. 19) constants and logarithmic bases are essentially arbitrary, so the relationships of eqns (36) and (44) ‘are identical’. To avoid any ambiguity, \( H \) in eqn (44) will be termed ‘Shannon entropy’.

### 6.3 Shannon Entropy

Assuming for the moment, the validity of the concept of ‘Shannon entropy’ we find the applications are wide-ranging indeed.

The following discussion relates to representative contemporary subject areas.

In engineering, the cost of manufacturing an item depends on its complexity, in the sense that a quantity of information is necessary to construct that item. Such information can also form an assessment of the capital and labour costs involved. On that basis Thoma ([23], p. 14) can compare the lifetime information for steam and diesel locomotion. Quantification of information – again identified with entropy – is also a characteristic of the comprehensive application of Brooks and Wiley [25] to the field of biology. Topics, with specific calculations, include DNA (pp. 118/119) and ontogeny (pp. 7), phylogeny (p. 189), cohesion of populations (pp. 212 ff.), speciation (pp. 232/233) and phylogenetic trees (pp. 234 ff., 273), food webs (p. 304) and ecology (p. 318, p. 340).

In complete contrast to engineering and science is art. Arnheim [26] gives an intensively argued explanation of the meaning of entropy within art in general. He sees (figure 10.2, p. 30) art as ‘structural order’ brought about by ‘two cosmic tendencies’. The structuring theme is achieved by an Anabolic Tendency, ‘which initiates all articulate existence’, with the ordering achieved by a Tension Reduction Tendency organizing energy in ‘the simplest most balanced’ manner. In addition, entropy provides a negative catabolic destruction and is the partial (?) cause of tension reduction. Thermodynamicists would wince at all this (to put it mildly!) but the overall argument could possibly be rewritten in a more rigorous manner.

Our final representative study is that of Goonatilake [27] who focuses on information ‘flow lines’ in DNA, neural-cultural systems and then artefacts (cover blurb). The climax of his treatment is the
presentation of world history as a series of bifurcations (pp. 155–162), i.e. as a chaotic system.
The chapter in question, rather esoterically entitled ‘The deep engines of entropic change’, is
largely inspired by the work of Shannon, Prigogine, and Brooks and Wiley (pp. 140–151).
Space does not allow discussion of the interpretation of other areas in entropic terms, such as
economics (extensively referenced by Goonatilake, p. 152).

6.4 Dissipative structures

This entropic approach, stemming from the second law of thermodynamics, is by no means as
revolutionary as might be thought. It should be regarded as a sub-set of the relevance of thermodynamics
to these subject areas. This is clear from two other recent authoritative publications,
which coincide with [28] or overlap [29] Goonatilake’s interests. Both have detailed reference
to energy (hence first law) considerations ([28], pp. 95–97, 193 ff.; [29], pp. 69 ff.). The point
of our chapter is that second law considerations are equally significant, and in particular the
developments in non-equilibrium thermodynamics associated with Prigogine. These especially
apply to living systems, as noted in Section 1.

Such systems maintain their existence by consuming free energy (Schrödinger’s negative entropy)
from their surroundings. They export entropy to their surroundings via chaotically
oriented dissipative processes. The supreme example is the closed system of the biosphere, which
receives low-entropy energy from the sun, and dissipates high-entropy energy in the form of
radiation into space. Simple energy considerations lead to a bottom–up interpretation of organic
activity via the food chain, whereas the overarching historical biosphere effect is more of a
top–down low entropic driving force.

Once again an excellent summary of the whole material of this chapter, and its inclusion in a
cosmic ‘programme’, is given by Chaisson [16].

7 Pros and cons of Shannon entropy

7.1 Introduction

It is of crucial interest to establish whether the information-based Shannon entropy may be
identified, via statistical entropy, with the thermodynamics-based thermal entropy. Three levels of
comparison may be distinguished: prima facie, formal thermodynamics and universality of the
second law of thermodynamics. The first tends towards identification, the second and third
against.

7.2 Prima facie comparison

This arises from the complete similarity of form of eqns (44) and (36) for Shannon and statistical
entropy respectively. Moreover, the underlying concepts of thermal and Shannon entropy are
negative in quality: ‘disorder’ or ‘diminution of potential’ (constraints; [10], p. 18) in the case of
entropy, ‘uncertainty’ in the case of information. This argument is even finer when Shannon and
statistical entropy are compared: ‘uncertainty’ is an acceptable expression for both. In fact (as
explained later) Tribus structures his entire thermodynamic approach on the basis that entropy
and uncertainty are coincident ([30], p. 77).

Further, in eqn (45), the positive quality ‘information’, in the sense of removal of uncertainty,
has given rise to negentropy as a defined property.
7.3 Formal thermodynamics

This practice is not to be recommended.

J.D. Fast [31], p. 330

… there are in science today two ‘entropies’. This is one too many.

Jeffrey Wicken [10], p. 23

A typical selection of recent thermodynamics texts [11, 32, 33] avoids this issue completely. Further, they almost avoid the statistical definition of entropy itself. Out of the over 1500 pages in [11, 32, 33] there are only Winterbone’s sentence that ‘… statistical mechanics and the kinetic theory … do not give a good macroscopic theory of … (irreversible) processes’ ([32], p. 316), and Kondepudi and Prigogine’s page ‘Statistical Interpretation of Entropy’ ([33], pp. 91/92). The reader should not interpret our comment as in any way pejorative, but rather note that there is something unusual about thermodynamics to allow such an omission. Further, while the (again recent) specialised discussion of entropy by Dugdale [34] indeed treats statistical entropy, still the issue of Shannon entropy is not addressed. However, we do find ‘Entropy and information’ discussed in Fast’s older study of entropy ([29], pp. 325–332).

Fast’s essential conclusion is that Shannon entropy and conventional entropy are not connected at all (‘are two entirely different concepts’, p. 332) and any similarity starts and ends with the equations we have quoted. His arguments consist of a range of anomalies, including what he terms an ‘absurd result’ (p. 330) in trying to make a thermal equivalent to information. It is little wonder that ‘this practice is not to be recommended’ (p. 330) in his view.

Wicken is more sympathetic than Fast, because he uses information theory as an integral part of his overall explanation of evolution. Fast dismisses negentropy as a concept, describing the italicised statement of Brillouin ‘Any additional piece of information increases the negentropy of the system’ as a ‘tautology’ (p. 331). Wicken, on the other hand, uses it, but redefined as complexity. ‘There is a completely appropriate alternative to “entropy” in information theory. This is “complexity”.’ ([10], p. 24), leading to his grand biological statement: ‘This ordered, information-rich, and negentropic complexity lies at the heart of biological organization’ ([10], p. 49).

Returning to the question of Shannon entropy, Wicken’s conclusion is the same as Fast’s – ‘… two “entropies” … one too many’ ([10], p. 23). He wants to ‘expunge “entropy” from the lexicon of information theory’ ([10], p. 27). In support of this, he adduces a series of inconsistencies in the rationales for the two entropies ([10], pp. 19f). Now these inconsistencies can be more subtle than Fast would allow. In discussing the application of the two entropies to the crucial thermodynamic concept of path-independent changes of state ([10], pp. 22/23), Wicken admits his own confusion in the past: … ‘not been exempt … this loose language …. ‘ ([10], p. 23).

So formal thermodynamics refuses to mix with Shannon entropy. Does this mean that the entire enterprise of Brooks and Wiley ‘Toward a Unified Theory of Biology’ [25], Subtitle, is thereby invalidated? We turn now to the wider question of the universality of the second law of thermodynamics.

7.4 The second law of thermodynamics

The second law of thermodynamics is not restricted to engineering. It is a fundamental law of nature … biological organisms fully comply with the second law of thermodynamics.

Paul Davies [17], pp. 27/30
The ubiquitous second law of thermodynamics … is degrading the energy in the food chain at each link.

John Barrow [29], pp. 69/70

For each structure (sun, earth’s climasphere, biosphere, hominid body, human cranial, modern culture) the entropy increase of the surrounding environment can be mathematically shown to exceed the entropy decrease of the system per se, guaranteeing good agreement with the second law of thermodynamics.

E.J. Chaisson [16], p. 18

Since the Second Law governs all irreversible processes, a materialistically coherent cosmos requires their connection.

Jeffrey Wicken [10], p. 6

The above quotes, which omit any from Brooks and Wiley themselves, almost write this section. The mainstream conclusion is clear – the second law is universal in its applicability. What of the approach of Brooks and Wiley? The second law is indeed relevant (as working systems, organisms are subject to the second law of thermodynamics ([25], p. 33)), but that law is only a part of the story. ‘… this is not enough’ (p. 9). Yes, energy considerations are valid for living organisms ‘just like steam engines’ but ‘strictly thermodynamic considerations are not likely to tell us much …’ ([25], p. 33). No, ‘information takes precedence over energy’ (p. 34), so their second law is the second law of (information, energy …) and correspondingly their entropy relates to (information, energy …). ‘We are able to see biological evolution and thermodynamic changes as special cases of a more general phenomenon of evolution. … The second law is more than the natural law of energy flows; it is the natural law of history’ ([25], p. 355/356). Employing HIT (hierarchical information theory ([25], p. 71)) leads to ‘The total information capacity of the system is equivalent to the total entropy ($H_{\text{max}}$) of the system’ (p. 72). As a consequence, as neatly summarised by Goonatilake ([27], p. 150), ‘they show that biological systems are entropy-increasing with respect to themselves even though they would appear to an outside static observer as entropy-reducing’. This is because Brooks and Wicken distinguish between a static observer and one ‘perched on the line that represents entropy maximum’ ([25], p. 39).

Allied to this is disagreement with Wicken over ‘negentropy’. The latter uses ‘the “negentropy” concept … to express the idea of “probabilistic compression” of distance from equilibrium’ ([10], p. 36). Moreover ‘negentropic complexity lies at the heart of biological organization’ ([10], p. 49). For Brooks and Wiley, however, even if the entropy of living systems doesn’t ‘increase’, this does not mean that (they) are in any sense ‘negentropic’ ([25], p. 355). But, of course, the meaning of ‘negentropic’ for Brooks and Wiley must be affected by their understanding of entropy itself.

Since the missions of Wicken and Brooks and Wiley are largely coincident, and ones with which we have great empathy, differences of this kind are unfortunate.

It has to be noted that Brooks and Wiley misunderstand certain thermodynamic issues. For example, on p. 7 they say that the (enthalpy-based) Gibbs free energy $G$ was formulated for use with closed systems. In fact it is the brother function $F$, the (internal energy based) Helmholtz free energy that is tailored to closed systems. The distinction is clear, for example, in non-flow and flow combustion situations which must use internal energy and enthalpy, respectively, as the basis for caloricific values of fuels. Of course, once defined as a thermodynamic property $G$ is automatically quantified by the thermodynamic state of the system. Nevertheless, it is the (Gibbs) free energy that ‘feeds’ the living systems, as all other authors attest.
More significant, however, are their comments on Prigogine’s equation (pp. 9 and 57). They indeed recognise it is for open systems, but say it ‘neglects the state of the system itself’ (p. 9), and ‘does not address the very attributes of biological systems that suggest thermodynamic behaviour’. Despite what Brooks and Wiley appear to believe, the energy cost in bringing particles into the system, is indeed allowed for in enthalpy-based analyses. While the state itself does not explicitly appear in the Prigogine equation, it is changes in state that most thermodynamic equations relate to. Further, they state that ‘We do not assert that energy flow is trivial, only that there is no external energetic imperative behind organismic diversification’ (p. 34). This is inconsistent with other authors, e.g. ‘The biosphere … trapping radiant energy … necessarily provides riches in which AOs can emerge and evolve … the generation of structure: from molecular complexification to microsphere formation’ ([10], p. 117). Doesn’t this constitute some form of imperative?

Despite all the above, Brooks and Wiley’s ‘alternative general mechanism for driving systems’ (p. 58), which directly relate to expanding phase space cosmological models, has an inherent attractiveness, and later we will return to this point.

Finally, Brooks and Wiley stress the difference between closed and open systems. For a biological (open) system their entropy would increase, but by less than it would for a closed system by virtue of some ‘entropy production … dissipated into the surroundings’ ([25], p. 9).

Now an engineering approach to an issue such as this postulate would be to identify some limiting case which has least uncertainty. Since the biosphere is a closed system (‘the biosphere as a whole is the ultimate unit of cyclic closure’ ([10], p. 146)) then Brooks and Wiley’s above entropy reduction would be made zero. From that viewpoint, it is advantageous that Wicken studies the biosphere, and, moreover, that the ensemble statistics of thermodynamics can be applied in their theoretical microcanonical form ([10], p. 34). Conversely, it is somewhat disappointing that Brooks and Wiley do not consider biosphere processes.

7.5 The thermodynamics of Tribus

Finally, there is Myron Tribus’s complete re-description and exhaustive treatment of thermodynamics in terms of information theory. Tribus took the Shannon information equation (44) as a basis, with \( S \) formally defined as both the entropy and uncertainty ([30], p. 77). Applying this to the statistics of a perfect monatomic gas allowed him firstly to explain temperature, thermal equilibrium and the zeroth law of thermodynamics (pp. 117–119), then heat, work and the first law (pp. 124–140), and finally ‘classical’ entropy and the third and second laws (pp. 140–145). It is presented as an undergraduate course text, with the explicit support in 1961 of L.M.K. Boelter, Dean at UCLA, ‘who never doubted that the junior-year students could master this material’ (p. ix). The rationale for this radical approach is of considerable interest, as it follows E.T. Jaynes (see p. viii) who ‘took the ideas of information theory as primitive and more basic than thermodynamics’.

The question of the validity of Tribus’s approach – and behind it whether Jaynes’s assertion is justifiable – is now addressed. We have seen how reluctant thermodynamicists are to welcome Shannon entropy to their high table, and this is reflected in the total lack of mention of Tribus or Jaynes by either Rogers and Mayhew [11], Kondepudi and Prigogine [33] or Fast [31], for example. However, while Tribus majors on background information theory, in practice he confines his mathematical application to microstate statistics vis-à-vis Boltzmann. In so doing his rationale is implicitly accepted by Wicken, who at the same time as he refuses ‘Shannon entropy’ accepts ‘Jaynes’s approach’ ([10], p. 21).
Now this is consistent with the demonstration earlier in the present chapter that thermal and statistical entropies are equivalent. Classical thermodynamics is empirical in character: ‘the important fact that thermodynamics is essentially an experimental science. It is not a branch of mathematics’ ([11], p. 80). So, by demonstrating, as we have done, the equivalence of the two entropies, the Boltzmann statistical version is at the very least, established. Moreover, if such demonstration is extended to showing full coincidence of the two entropies, they then become equally and independently valid. Fast ([31] p. v), supports this: ‘the two methods provided by thermodynamics and statistical mechanics’. Tribus and Jaynes, or more correctly, Jaynes and Tribus, take this logic several crucial stages further. Firstly, they adopt the Shannon information theory as a rationale which provides a definition of entropy as ‘uncertainty’ ([30], p. 77). They do this in a sufficiently carefully applied manner to be acceptable to Wicken ([10], p. 21), and to others. Their ‘uncertainty’ is microscopically oriented. So we do find Tribus’s publications referenced by Wicken ([10], p. 232), by Brooks and Wiley ([25], p. 394) and by Winterbone ([32], p. 367). Secondly, Jaynes makes the almost revolutionary assertion of the primacy of information theory. Finally, Tribus restructures the whole thermodynamic enterprise from this direction. Unquestionably, it is mathematically oriented. Tribus, then, gives an alternative approach to teaching thermodynamics, and in fact at City University, London, UK, a colleague of one of the authors, Prof. I.K. Smith, used it as the thermodynamics section of a taught Master’s course for some years, in which M.W.C. participated. Furthermore, given the accepted applicability of thermodynamics to biology, it underlines the message of this chapter that the connection of energy with information in a biological context needs full exploration. As Wicken points out, however, what is meant by information requires careful understanding. Brooks and Wiley assert the prior status of information theory – ‘information takes precedence over energy when we consider the impact of the second law of thermodynamics on organisms’ ([25], p. 34). However, they mean what they describe as ‘instructional information’ rather than the statistically based view of Jaynes. Broadly speaking, it is a macroscopic/microscopic contrast, but even this cannot be used in a trite manner.

7.6 Conclusion

We conclude, therefore, that it is safer not to take ‘Shannon entropy’ as a valid direct equivalent of thermal or statistical entropy. Despite this, the whole enterprise of Brooks and Wiley is otherwise most satisfying, with careful quantification for all applications, and consistency with conventional biology. In concluding Chapter 4, Populations and Species, they note (p. 255) ‘the most startling and most hopeful outcome of this chapter is the recognition that the empirical core of neo-Darwinism, namely population biology, can be accommodated within our theory’. Setting aside the problem of entropy definition, there is a rather fine qualitative description and graph of varying biological timescales and ‘production’ effects (p. 372) and referring back (pp. 85/86). Their key scientific foundation is mainstream, namely the expansion of the universe and gravitational concentration of matter (p. 58). Finally, various information-related terms such as disorder/order (p. 69) and diversity, stability and evenness (p. 309), give scope for quantitative assessment of biological processes. Later in the chapter, we will give a comparative synthesis of the biological topics covered by them and by Wicken.

The debate has not gone unnoticed. Ji adopts a compromise ([36], p. 123). Like Brooks and Wiley, he uses H as the symbol in the Shannon equation and calls it entropy. However, he interprets it as complexity!
8 Information and complexity

There is a completely appropriate alternative to ‘entropy’ in information theory. This is ‘complexity’. … The Shannon ‘entropy’ of a sequence is simply the minimal program of information required for its specification.

Jeffrey Wicken [10], p. 24

A Shannon measure … is also a measure of complexity. …

D. Brooks and E.O. Wiley [25], p. 41

The complexity, or number of bits of information. …

Stephen Hawking [37], p. 163

8.1 Introduction

Complexity itself is a field of considerable current interest, but we will focus on the narrow issue of quantitative meaning of the Shannon equation. The treatment is concise as it lacks controversy.

8.2 Information

The Shannon and Weaver System does not allow for the semantics of information, its context or its meaning, a failing admitted by the founders themselves.

Susantha Goonatilake [27], p. 13

There is some ambiguity about the meaning of information as defined by the Shannon equation. The information specialist W. Gitt gives an incisive – if now possibly needing updating – analysis of the overall problem. He points out ([38], p. 36) that ‘Shannon completely ignores whether a text is meaningful, comprehensible, correct, incorrect or meaningless’. He addresses the issue by defining five levels of information – statistics, syntax, semantics, pragmatics and apobetics (or purpose) – supported by 14 theorems. (This paper is interesting also for its comparison of 1989 computer chips with DNA on the basis of information per unit volume. Also, estimating the total world knowledge in libraries as $10^{18}$ bits, in DNA molecule storage terms 1% of a pinhead volume would suffice ([38], p. 38)). Gitt’s reasoned criticism only mirrors the problems of definition. For example, admittedly in the context of complexity, Gell-Mann discusses AIC (algorithmic information content) [39]. He points out its unsuitability ‘since the works of Shakespeare have a lower AIC than random gibberish of the same length that would typically be typed by the proverbial roomful of monkeys’. Goonatilake’s quote summarises the above.

8.3 Complexity

For our purposes, it is sufficient to note the wide attention being currently given to the concept of complexity and complex systems. Typical of authoritative substantial publications are (also giving subtitles) Exploring Complexity – An Introduction by Nicolis and Prigogine [40], Complexity – Life at the Edge of Chaos by Lewin [41], and At home in the Universe – The Search for the Laws
8.4 Quantification of complexity

As Gell-Mann points out [39] ‘a variety of different measures would be required to capture all our intuitive ideas about what is meant by complexity’. His criticism of AIC has been noted, just as Shalizi [45] highlights Kolmogorov’s measure ‘as useless for any practical application’. To hand is a research paper studying mathematical models for the complex dynamics of fisheries, and the chronic problem of over fishing (Of fish and fishermen: models of complexity [46]). These models comprise neoclassical equilibrium approach and system dynamics in the context of the Canadian Atlantic coast.

8.5 Conclusion

In contrast to Shannon entropy, the identification of the Shannon function with a quantitative measure of complexity finds Wicken, Brooks and Wiley, and Ji in accord. Moreover Hawking’s terse comment is actually biological: ‘the complexity, or number of bits of information, that is coded in DNA is roughly the number of bases in the molecule’. Also, this quite straightforward definition has a parallel in Thoma’s application of Shannon’s formula to complexity/information for capital/labour/specification in a mechanical engineering context ([23], p. 11).

Finally, since Brooks and Wiley’s calculations are Shannon based, a large reconciliation is possible by using the term complexity, rather than entropy, that is to say ‘Evolution as complexity’ as an alternative title.

9 Evolution – a universal paradigm

… what Darwinism does for plants and animals, cosmic evolution aspires to do for all things.

Eric Chaisson [16], p. 14

… the cosmological evolution, including the evolution of living systems. …

Sungchul Ji [36], p. 156

… evolutionary processes in three discrete domains. These domains are biology, culture and man-made information systems.

Susantha Gonatilake [27], p. 1

Last but not least, the universe as a whole is continuously evolving.

Grégoire Nicolis and Ilya Prigogine [40], p. 37
9.1 Introduction

In certain respects, this section forms the climax of our chapter. In it we discuss the generalisation of the evolutionary rationale to 'all things' (above quote), the underlying driving forces of gravity and the expansion of the universe, and the key roles played by thermodynamics and information/complexity. The issues are well illustrated by alternative graphical presentations, redrawn from the works of a number of authors.

9.2 The expansion of the universe and its gravity

... a veritable prime mover ... is the expansion of the universe itself.

Eric Chaisson [16], p. 13

The most important fact about the universe today is that it is expanding.

John Gribbin [44], p. 111

Looking at the universe as a whole ... arranged itself into shining proto-galaxies ... the expansion of the universe assisted ... an entropy gap opened up ... all sources of free energy ... can be attributed to that gap. ... The ultimate source of biological information and order is gravitation.

Paul Davies [17], p. 41

... the evolution of the cosmos ... there has existed an asymmetry between potential and kinetic forms of energy due to cosmic expansion, which makes descents into potential energy wells entropically favourable ... constitute means for the dissipation of potential energy.

Jeffrey Wicken [10], p. 63/64

It is part of the challenge of our overall study, but also part of its satisfaction, that the entire biological enterprise rests on the secure scientific foundation of the nature and history of the universe. Not only that, but such a foundation is, almost by definition, a thermodynamic one, as our quotes make clear. That history is given in display form by, for example, Rees ([47], p. 119) and Hawking ([37], pp. 168/169) with (p. 78).

The next key event to follow the Big Bang was the decoupling of matter and radiant energy, completed after around 100,000 years. Figures 4 and 5, redrawn from [16], display the processes quantitatively. Following this decoupling the temperatures diverge, and result in the inception of information/complexity as explained by Chaisson.

An extended alternative to Figs 4 and 5 is presented qualitatively in Fig. 6, in three-dimensional form (redrawn from [36], p. 156).

In Fig. 6, $E$ represents qualitatively the energy density of the earth so is somewhat more specific than Fig. 4. Also, the information density $I$ represents only biological information, as opposed to the overall cosmic information of Fig. 5b which increased from zero after decoupling. Ji also postulated a possible non-zero information content of the universe at the time of the Big Bang which (despite 'probably varying with time', Ji, figure explanation, ([36], p. 156)) is represented as a constant thickness in the $I$ direction.

The overall message is clear and presented by both authors in an essentially consistent manner. Chaisson’s concise accompanying description, which stresses the thermodynamics ([16], p. 16) is complemented by that of Davies ([17], pp. 37–41), who explains the thermodynamic consequences...
The Laws of Thermodynamics

Figure 4: Variation of energy density of matter and radiation. The lines cross at about 10,000 years, one-tenth of the time taken to fully decouple matter and radiation (redrawn from [16]).

of gravity. Figure 5b reflects the ‘virtually informationless’ character of the originally ‘undifferentiated and highly uniform blob of plasma’ (Chaisson) – or the ‘very little information’ of the ‘uniform gas’ (Davies). Figure 5b also reflects the commencement of cosmic information due to the concentration of matter. ‘A smooth gas grows into something clumpy and complex’ – ‘a star cluster or a galaxy requires a lot of information to describe it’ (Davies).

The existence of gravity provides a key to the cosmic thermodynamic enterprise. ‘In the 1980’s’ (Davies explains) ‘the puzzle of the source of cosmic energy was solved’, ‘because its gravitational field has negative energy’. Also ‘the universe came stocked with information, or negative entropy, from the word go’. In the context of our post Big Bang plasma/gas ‘a huge amount of information evidently lies secreted in the smooth gravitational field of a featureless, uniform gas’.

So as the cosmic matter/radiation system evolves, information emerges, and a cosmic entropy gap opens up – the difference between the maximum possible entropy and its actual entropy.

There is therefore a cosmic entropic driving force with the objective of raising the universe’s actual entropy to its maximum – in other words, the second law of thermodynamics. The thermodynamics of our earth is part of this cosmic mission. Although in energy terms, ‘the earth sends back into space all the energy that it receives from the sun’, in entropy terms, the energy ‘we do receive has a far lower entropy than the (equal) energy that we return’, to give Penrose’s simple yet telling explanation (Introduction ([6], pp. xi–xii)). Whether concerning our chemical or geothermal energy, or – specifically for this chapter – ‘biological information and order’, ‘the ultimate source is gravitation’ ([17], p. 41).

The effect of cosmic expansion gives the ‘ever-widening gradient of the universe’s ‘heat engine’ (([16], p. 17); Fig. 5) and so becomes ‘the prime mover’. Whereas for Davies the focus is on gravitation, there is no contradiction. In fact, Hawking ([48], p. 165) gives the same sequence as
Figure 5: Temperature variation of matter and radiation in the universe, leading to evolution of information, after Chaisson (Redrawn from [16] and quoting his comments in full.)

(a) The temperature of matter and radiation went their separate ways once these quantities became fully decoupled at $t \approx 100,000$ years. Since that time, the universe has been in a non-equilibrium state – a kind of cosmic heat engine. (b) The potential for rising negentropy or information content – un-quantified here but conceptual synonyms for ‘complexity’ – is broadly proportional to the growing thermal gradient in the universe.

Davies, but with the stress laid on the cosmic expansion. So expansion and gravitation jointly form the cosmic fact of life.

Finally, like Davies, Chaisson is particularly attracted by ‘life forms’ which ‘arguably comprise the most fascinating complexities of all’ ([16], p. 16). As a consequence his cosmic history has only three eras, the radiation era and matter era (Fig. 4) now succeeded by the very recent life era – ‘the emergence of technologically intelligent life’ ([16], p. 17).

So the thermodynamics of the universe is identified with our current biological perspective.

9.3 The evolution of information/complexity

9.3.1 General

The preceding section focused on two major historical events, the decoupling of matter and radiation, of cosmic significance, and the origin of life on earth of biological significance.
Figure 6: Evolution of information, after Ji (redrawn from Ji). ‘The sudden increase in the information density (defined as the amount of biological information divided by the volume of the biosphere) occurred with the emergence of the first self-replicating systems in the biosphere on the earth about 3 billion years ago’ ([36], p. 156).

Figure 7: The components of cosmic evolution expressed as a function of their consumption of free energy. (Redrawn from [16] and quoting his comments in full.) The rise in free energy rate density, $F$, plotted as horizontal histograms for those times at which various open structures have existed in nature, has been dramatic in the last few billion years. The dashed line approximates the rise in negentropy, information, or complexity sketched in the previous figure, but it is energy flow, as graphed here, that best characterises the order, form, and structure in the universe. The three principal eras, discussed in this paper, are bracketed across the top.

In Fig. 7 Chaisson’s minimalist history of Fig. 5b is now detailed. Cosmic evolution results in negentropy/information/complexity residing in (a) ‘matter scattered throughout the universe’ in space, (b) biological structures, and (c) society. Moreover, it is not so much the output which can be quantified, as the rate at which free energy can be processed, as a kind of volumetric effectiveness.
This, we should be reminded, is the direct consequence of the free energy arising, from the entropy gap, and from which ‘all life feeds’ ([17], p. 41). It is all part of the grand entropic scheme, with the effectiveness of free energy consumption increasing substantially from stage to stage in the evolution.

Goonatilake has the same rationale. It is based on what we might now regard as the new Prigogine-oriented thermodynamic orthodoxy. ‘Free energy is continuously fed into the living system to balance the outflow into the environment occurring with the decrease in entropy owing to the increase in information. In the open systems of living organisms, entropy decreases with growing differentiation’ ([27], p. 14).

Furthermore, by combining ‘the living system and the environment’ Goonatilake correctly, and identically with Chaisson ([16], p. 18 and quoted previously) states that consistency with the second law is achieved, as ‘the entropy in the total system – of the living (organism) and its environment – increases’ ([27], p. 14).

Not only is the basis of Goonatilake’s and Chaisson’s studies entirely consistent, but so is their attitude to information. Goonatilake sees all information systems, whether they are purely biological, cultural or artificial (called ‘exosomatic’) as part of the same evolutionary stream. So the evolutionary phylogenetic tree is extended to include the other two information systems, as in Fig. 8.

Figure 8: Phylogenetic tree with cultural and exosomatic information systems (redrawn from figure 9.5 [27], p. 139.)
9.3.2 Cultural information

The only eucultural species is man

Susantha Goonatilake [27], p. 31

Using material from [49], Goonatilake presents the various grades of cultural evolution, and the number of species for each grade.

This material enables the (broken lines of) cultural evolution to be superimposed on the phylogenetic tree of Fig. 8, where the tree itself represents the evolution of genetic information.

It will be noticed from Table 3 how each new defined grade of culture results in a sharp reduction of number of species, until, at the eucultural level the only species remaining is man. Furthermore, man is also unique in developing Goonatilake’s ‘exosomatic’ or artificial information systems.

9.3.3 Exosomatic information

This is one of the principal themes of Goonatilake’s study [27], and is indicated in Fig. 8 as a region of evolution of information for Homo sapiens at the upper right of the tree. The region is in parallel, therefore, to the eucultural information. The exosomatic information stream commenced with writing (timescale \(\sim 4000\) years ago ([27], p. 130)) through printing (1457), steam printing

Table 3: Explanation of cultural evolution and corresponding species. (Redrawn from figures 4.2 and 4.3 [27], pp. 30–31; Lumsden and Wilson [49]).

<table>
<thead>
<tr>
<th>Components</th>
<th>Reification (including symbolization and abstract thinking)</th>
<th>Species density</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Acultural I</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Acultural II</td>
<td>●</td>
<td>All invertebrates and cold-blooded vertebrates, i.e. 1,000,000 species</td>
</tr>
<tr>
<td><strong>Protocultural I</strong></td>
<td>●</td>
<td>8600 species of birds and 3200 species of mammals</td>
</tr>
<tr>
<td>Protocultural II</td>
<td>● ●</td>
<td>Seven species of wolves and dogs, single species of African wild dog, one species of dhole, one species of lion, both species of elephant, 11 species of anthropoid apes</td>
</tr>
<tr>
<td><strong>Eucultural</strong></td>
<td>● ● ●</td>
<td>Man is the only species</td>
</tr>
</tbody>
</table>
(1814), still photography (1820), phonograph/telephone (1876) as typical landmarks, and is with us today in full flood with a plethora of computer-oriented systems. In parallel with this is an assessment of the information content – cuneiform tablet – $10^2$ bits, typewritten page – $10^3$ bits, magnetic tape – $10^6$ bits, and ‘ultrafine silver haloid film’ using an electronic microscope to generate microbeam storage – $10^{12}$ bits ([27], p. 95). A third aspect is the manner in which exosomatic information has grown, as plateaus but with each invention causing rapid growth – ‘rapid information growth with discontinuities’ is Goonatilake’s description ([27], p. 128). In fact, Goonatilake points out that it is a ‘similar phenomenon to punctuated equilibrium in genetic evolution’ (p. 68).

Omitting these discontinuities enables Fig. 9 to be constructed, as a qualitative description of the overall evolution of information since the origin of life on earth. Goonatilake’s model may be compared with that of Hawking ([37], p. 163), redrawn as Fig. 10.

Apart from Hawking’s omission of cultural information, the interpretation is essentially the same. Moreover, in the 10 years between their publication, the quantitative assessment of DNA has become clear, so Hawking can directly compare the ‘genetic’ and ‘exosomatic’ aspects of Goonatilake.

### 9.3.4 Genetic engineering

An extremely important issue for our discussion, is the feedback information loop which enables *Homo sapiens* to adapt its own DNA. ‘There has been no significant change in human DNA in the
last 10,000 years, but it is likely that we will be able to completely redesign it in the next thousand’ ([37], p. 165). He points out that this is a rational prediction, irrespective of ethical issues. ‘Unless we have a totalitarian world order, someone somewhere will design improved humans’. For Chaisson, this ‘feedback loop’ (our words) is a key aspect of his cosmic evolutionary scheme. ‘Technologically competent life differs fundamentally from lower forms of life … after more than 10 billion years of cosmic evolution, the dominant species on earth – we, the human being – has learnt to tinker not only with matter and energy but also with evolution. … We are, quite literally, forcing a change in the way things change’ ([16], pp. 16–17).

9.4 Time’s arrow

The increase of disorder or entropy with time is one example of what is called an arrow of time, something that distinguishes the past from the future.

Stephen Hawking [48], p. 161

The cosmological arrow generates randomness; the evolutionary arrow generates complexity and organization. We must connect the two.

Jeffrey Wicken [10], p. 77

When a process is always spontaneously irreversible, it can be said to have an ‘arrow of time’. … The arrow of time and the arrow of history for biology are complementary…

Daniel Brooks and E.O. Wiley [25], pp. 6, 63
The interface between thermodynamics and biology also requires an understanding of the concept of time. The second law with its entropy always tending to increase, means that that increase in entropy is also a marker of the passage of time, from past to future. For Brooks and Wiley, their ‘why’ of the ‘path to a more unified theory of biological evolution … must include the contributions of the only natural law with a sense of time’ ([25], pp. 50–51). For Goonatilake’s study of the evolution of information, it is the same. The second law ‘gives direction in time to physical processes, “the arrow of time” in the words of Arthur Eddington’, and ‘evolution as entropy in biology’ is followed by ‘historical change and entropy’, ([27], pp. 144, 147 and 156).

Here again we detect a common understanding of time as an arrow, and Chaisson uses it as a cosmic ‘intellectual road map’ ([16], p. 13), as shown in Fig. 11. Its content has already been largely discussed.

It is clear from the introductory quotes above that there is more than one arrow, and this issue is very well explained by Hawking ([48], Chapter 9) ‘The arrow of time’. ‘There are’, he says, ‘at least three different arrows of time … thermodynamic …in which disorder or entropy increases … psychological …we remember the past but not the future … cosmological …universe is expanding rather than contracting’ ([48], p. 161). The first two ‘necessarily point in the same direction’, because computational processes (equivalent as far as we know to thought processes) will always obey the second law of thermodynamics. Comparing the first and third is more subtle, but consistent with the sequence described by Davies. ‘The universe would have started in a smooth, and ordered state, and … during this expansion … would become lumpy and disordered as time went on. This would explain … the thermodynamic arrow of time’ ([48], pp. 165–166).

So, inherent in (the time direction of) the expanding universe is (the time direction of) the disordering process, hence the two arrows point in the same direction. It is the former that gives rise to Wicken’s ‘evolutionary arrow that generates complexity and organization’ ([10], p. 77). Moreover, Hawking’s three arrows point in the same direction and his argument is that it is only then ‘that conditions are suitable for the development of intelligent beings who can ask the question. …’ ([48], p. 161). This is connected with his discussion of the anthropic principle – termed ‘We see the universe the way it is because we exist’ ([48], p. 137 ff.). [The anthropic principle, finally, he connects with possible belief in a Creator – ‘One can take this either as evidence of a divine purpose in Creation and the choice of the laws of science or as support for the strong anthropic principle’ (p. 139). Although the ethos of this chapter, volume and series is to...
be neutral on such issues, they tend to appear consistently, and could form an attractive extension of our study. Frequently, the authors of our references either implicitly or explicitly express their individual beliefs. M.W.C. writing as series editor.

A related issue could be mentioned in closing. It is the question of what would happen in a contracting or collapsing universe ([48], p. 166; [10], p. 78). Then, and in common with the behaviour of black holes, the cosmic and thermodynamic arrows would be opposite – ‘the thermodynamic and psychological arrows of time would not reverse when the universe begins to recontract or inside black holes’ ([48], p. 167). Wicken mentions a ‘devolutionary … arrow’ ([10], p. 78).

9.5 Conclusion – an evolutionary paradigm

This section, well epitomized by Chaisson, appears to concentrate all science, engineering and humanities into one space – cosmic evolution. We have shown that in fact the ground rules of this concentration are fairly few – the history of the universe and the laws of thermodynamics, especially the second. There is a fairly tight range of individual aspects – such as cosmic expansion – with a common interpretation. Authors have also presented the evolution of information graphically, and again such presentations are consistent.

Overall, this section reflects an emerging mainstream of thought on cosmic and terrestrial history.

10 Evolution of the biosphere

Such a thermal gradient is the patent signature of heat engine.

Eric Chaisson [16], p. 17

The source–sink dynamics is responsible for the energetic ‘charging’ of the prebiosphere prior to life’s emergence.

Jeffrey Wicken [10], p. 39

The biosphere has evolved over the ages … absorbing solar energy, chemically degrading radiant energy, and releasing thermal entropy to space.

Jeffrey Wicken [10], p. 39

… the evolution of the biosphere is manifestly a physical process in the universe…

Stuart Kauffman [50], p. 245

10.1 Introduction

The history of the prebiosphere/biosphere is the primary key to uniting thermodynamics with biology. Embedded within the cosmic evolutionary programme are two high temperature (low entropy) sources of energy, earth’s mantle and the sun. These provide a top–down driving force for the eventual emergence and development of life forms. The processes are especially addressed by Wicken [10].
10.2 The biosphere

As a working definition Wicken uses ‘not only the blanket of living things that covers the earth, but also the abiotic matrices in which they live – which include the atmosphere and geochemical stores with which they exchange materials and energy. The biosphere as a whole is a closed thermodynamic system, cycling elements and irreversibly processing energy’ ([10], p. 74).

This is quite close to a typical ‘popular’ encyclopaedic definition: ‘that region of the earth’s surface (land and water), and the atmosphere above it, that can be occupied by living organisms’ [51].

A somewhat weaker definition is provided by the exhaustive undergraduate biological text *Life* ([8], p. 8). ‘Biological communities exchange energy with one another, combining to create the biosphere of earth.’

The question of precise definition has a direct relevance, for example, to Lovelock’s ‘gaia’ concept [52]. It is hoped to review this, in the thermodynamic terms of this chapter, in a future volume of the Series.

Further, the energy issues on which Wicken and ‘Life’ focus above are comprehensively identified by Barrow ([29], pp. 69–70). The issues form the background to a fascinating and quantitatively well informed discussion of the weight, size, complexity, population density and brain size of various species ([29], pp. 68–86). For Barrow, the second law is ‘ubiquitous’, degrading ‘the energy in the food chain at each link’ (pp. 69–70).

10.3 The thermodynamic model

10.3.1 The terrestrial heat engine

Under the heading ‘Sources, Sinks and Energetic Charging’ ([10], p. 70), Wicken describes the charging of the prebiosphere to ‘higher levels of free energy’ and how, by dissipating that free energy ‘molecular complexity’ was ‘generated’. Assembling the various components, the thermodynamic activity may be visualised as a kind of terrestrial heat engine, but with no work output. Figure 12 gives the two cases of geothermal and solar heating.

There are subtle differences, however. In an engineering heat engine, the thermodynamic state of the system itself varies cyclically, and $Q_1 > Q_2$, with $Q_1 - Q_2$ being the work output. In the case of the prebiosphere, $Q_1 > Q_2$, but the inequality results in a ‘charging’ of the system.

Figure 12: The terrestrial heat engine dominant for (a) prebiosphere and (b) biosphere.
In the case of the biosphere, we have noted [6] that currently \( Q_1 = Q_2 \). Elsewhere, Wicken ([10], p. 146), points out that ‘since irreversible flows of energy through closed systems require cyclic movements of matter’ there is a strong cyclic character to the biosphere. For the prebiosphere, there is a drive towards such cycling.

Using the standard approach of Prigogine (eqn (3), but as expressed by Wicken ([10], p. 70)) for either an open or a closed system the change in entropy for the system \( \Delta S \) is given by:

\[
\Delta S = \Delta S_i + \Delta S_e, \tag{46}
\]

where \( \Delta S_i \) is the change within the system due to its internal irreversibilities, the second law requiring \( \Delta S_i > 0 \), and \( \Delta S_e \) is the net exchange with the environment.

From Fig. 11 (or the engineering equivalent ([9], figures 8 and 9, pp. 38–39)) the second law Carnot inequality is:

\[
\frac{Q_2}{T_2} - \frac{Q_1}{T_1} > 0, \tag{47}
\]

where

\[
\Delta S_e = \frac{Q_1}{T_1} - \frac{Q_2}{T_2}, \tag{48}
\]

giving

\[
\Delta S = \Delta S_i + \left( \frac{Q_1}{T_1} - \frac{Q_2}{T_2} \right), \tag{49}
\]

enabling \( \Delta S < 0 \), i.e. ‘a necessary condition for evolutionary self-organization’ ([10], p. 71). However, it is not a sufficient condition. The prebiotic evolution leading to emergence involves ‘chemical potential and molecular complexity’ (p. 71). This sequence also necessitates the ‘penetration of (solar) energy so that at certain points \( Q_1 \) exceeds \( Q_2 \)’ (p. 71).

This local penetration is the bottom–up prebiosphere driving force, complementary to the overall heat engine model. Wicken re-expresses \( Q_1 \) and \( Q_2 \) locally, so a kind of micro heat engine is driven by:

\[
\Delta H_s = (Q_1 - Q_2)_s. \tag{50}
\]

Correspondingly, a local geothermal driving force is provided by the identity \( \Delta H = \Delta G + T \Delta S \), where \( \Delta G \) is the Gibbs free energy, resulting in:

\[
\Delta H_g = (Q_1 - Q_2)_g = (\Delta G + T \Delta S)_g, \tag{51}
\]

where subscripts ‘s’ and ‘g’ refer to solar and geothermal respectively.

10.3.2 The growth of information

… the randomizing directive of the second law begins to make contact with the integrative movement of evolution.

Jeffrey Wicken [10], p. 76
This is based on information theory in the sense of statistical mechanics, and not on Shannon-type information. So macroscopic information \( I_M \) refers to a macrostate, the summation of ‘microstates contributing to that state’ ([10], p. 74). Specifically \( I_M \) ‘is related to the probability of the macrostate’s occurrence’ (p. 74). Omitting the underlying statistically related mathematics, and with \( I = -S \) as a basic relationship, \( I_M \) is given by:

\[
I_M = I_c + I_{th} + I_e, \tag{52}
\]

where \( I_e \) is the energetic information, \( I_e = E/T \) (\( E \) is the internal energy and \( T \) is the temperature); \( I_c \) is the configurational information, the overall probability of the ‘spatial configuration’ of the constituents and \( I_{th} \) is the thermal information, the overall probability of ‘allocation of kinetic energy among their … quantum states’ ([10], p. 75).

Wicken then divides ‘the universe’ (\( u \)) (p. 75) into the ‘limited system under consideration’ (\( s \)), and an infinite-capacity reservoir (\( r \)) ‘with which \( s \) can exchange materials and energy’.

With \( \Delta S \) representing a change in entropy, the second law can be expressed as:

\[
\Delta S_s = \Delta S_k + \Delta S_r > 0. \tag{53}
\]

Now

\[
\Delta S_s = - (\Delta I_c + \Delta I_{th}),
\]

and with no work output from \( s \),

\[
\Delta S_t = (Q/T)_s = - \Delta E/T = - \Delta I_e.
\]

The second law requirement then becomes:

\[
\Delta I_c + \Delta I_{th} + \Delta I_e < 0. \tag{54}
\]

This is a significant equation, as it re-expresses the second law entirely as changes of information, where ‘information’ is interpreted in microscopic/statistical terms. (To digress somewhat, Tribus [30] uses the entropy to information conversion in reverse, in his formulation of the laws of thermodynamics we considered earlier).

Equation (54) enables Wicken to explain the core of a thermodynamic understanding, based on statistical considerations, of prebiotic history. Growth in prebiotic complexity requires an increase in \( I_{th} \), i.e. in overall structuring, since structuring requires the ‘movement’ of thermal energy from practically continuous translational modes to much less densely spaced vibrational modes … reductions in kinetic freedom … hence reductions in thermal quantum states ([10], p. 76). \( \Delta I_{th} \) is given by:

\[
\Delta I_{th} < - \Delta I_c - \Delta I_e. \tag{55}
\]

This relationship expresses the thermodynamic constraints which allow ‘evolutionary complexification’ to occur.

Summarising, Wicken mentions two prebiotic effects:

1. formation of water from hydrogen and oxygen (\( I_{th} \) and \( I_c \) increase);
2. conditions in the atmosphere and oceans (\( I_{th} \) increases, \( I_c \) and \( I_e \) decrease).

However, he focuses on solar radiation, which provides increasing \( I_e \). Pointing out that \( I_e/I_{th} \) changes tend to be reciprocal, this gives:

3. solar radiation, increasing \( I_e \), then reducing \( I_e \), with increase in \( I_{th} \).
10.3.3 The arrow of time

The cosmological arrow generates randomness; the evolutionary arrow generates complexity and organization. We must connect the two.

Jeffrey Wicken [10], p. 77

Wicken points out that the second law does not ‘mandate directional changes in complexity with time. All it mandates are expansions in probability space’. However, the route of any process is constrained by the local prebiosphere conditions.

Hence the overall increase in ‘randomness of matter – energy in the universe’, causing $I_e$ to increase, is followed by the locally constrained and irreversible conversion of $I_e\rightarrow I_{th}$. This is shown in Fig. 13.

Also, he shows that ‘matter-randomization promotes …reactions essential to molecular evolution’, even in the absence of energetic charging. For these reactions, $I_{th}$ and $I_e$ are approximately constant, but the overall probability, $I_m \approx I_e$ becomes negative – ‘a highly creative force’ (pp. 79, 80).

Finally, Wicken lists the various stages of prebiotic evolution.

1. formation of simple molecules,
2. formation of biomonomers (amino acids, sugars, etc.),
3. formation of biopolymers (polypeptides, nucleic acids),
4. aggregation of biopolymers into microspheres,
5. emergence of ‘protocells’.

While the first four stages ‘can be understood straightforwardly’ from the preceding, the last ‘crucial’ step is the ‘most difficult to explain’ ([10], p. 81) Wicken addresses it in Part III of [10].

Our summary, due to lack of space, must finish at this point. There remain life’s emergence and Darwinian evolution to consider, which are addressed jointly in the next section.

Figure 13: The arrows of time in the prebiosphere – the growth of thermal information under the prebiosphere’s source–sink gradient (redrawn from [10]).
11 Thermodynamics, life’s emergence and Darwinian evolution

… a description in which evolution and history play essential roles. For this new description of nature, thermodynamics is basic. This is our message to the reader.

Dilip Kondepudi and Ilya Prigogine [33], p. xvii

We shall travel together through thermodynamics and biology.

Enzo Tiezzi [35], p. VIII

This book is written partly as a research program for bringing the mainstream of thermodynamic and statistical–thermodynamic thinking conservatively into evolutionary theory.

Jeffrey Wicken [10], p. 7

In this book we will develop the idea that evolution is an axiomatic consequence of organismic information and cohesion systems obeying the second law of thermodynamics in a manner analogous to, but not identical with, the consequence of the seconds law’s usual application in physical and chemical systems.

Daniel Brooks and E.O. Wiley [25], p. xi

11.1 Introduction

It may have been true in the past that ‘thermodynamics has been an uninvited guest in evolutionary discourse’ ([10], p. 7), but this is no longer the case. The objectives of the above four books make this clear. Like Wicken, our aim is to focus on mainstream thermodynamics, which includes consistency with Prigogine’s analyses. It is also apparent from the start that the approach of Brooks and Wiley differs somewhat.

In this section, we cannot hope to do other than provide a skeleton of the material presented as two entire books (by Wicken and by Brooks and Wiley) and other extensive writing (especially by Ji and Kauffmann). On closer analysis, we will find that the approach of Brooks and Wiley is representative of a much wider emerging unity. Three key themes are present in the living systems we now have to consider:

thermodynamic input, i.e. Gibbs free energy, output, or information/complexity, and internal behaviour of the system.

The fundamental issue is ‘What is life?’. This will lead to the question of life’s emergence, and thence to Darwinian evolution.

11.2 What is life?

What is life?

Erwin Schrödinger, Title of book [5]

What is life?

Jeffrey Wicken, Title, Chapter 2 [10]
... a proper definition of life itself ...

Stuart Kauffman, [50], p. 72

... what distinguishes life from nonlife ...

Sungchul Ji, [36], p. 99

... the riddle of life.

Ilya Prigogine, Chapter title [7]

To consider such a weighty question as ‘What is Life?’ is like climbing a whole mountain of perception. The reader may expect the view from the top should have an intellectual grandeur to reward the effort involved. Such is provided, we feel, by Kauffman ([50], p. 47), ‘… that mysterious concatenation of matter, energy, information and something more that we call life’. In keeping with our aim of defining the common ground, we have analysed a number of models in some detail. We find two principal features, those of thermodynamics and information.

Table 4 shows a synthesis of five relevant models, which, when further grouped into input – activities – output, show remarkably close agreement. The thermodynamics aspect is virtually coincident, the question of Kauffman’s work cycle being held over to the ‘fourth law of thermodynamics’ discussion in Chapter 6. The information aspect, although more patchy, is hardly less in agreement. In fact the overall models of Wicken and Kauffman barely differ. Kauffman stresses the autonomous agent activity, but so does Wicken’s ‘AO’ or autocatalytic organization ([10], p. 17); also both involve reproduction as an additional function.

Are these two aspects of thermodynamics and information competitive? No, for Wicken ‘the informational dimension of life is incorporated with its thermodynamic identity, but not conflated with it’ ([10], p. 31). In fact, an extended third quote from Wicken rather elegantly encompasses Table 4 ([11], p. 25). ‘Complexity and entropy have complementary significances in the emergence and evolution of life. The production of one, and its dissipation to the sink of space, provides the driving force for the biosphere’s complexification and generation of thermodynamic potential; the creation of the other through these negentropic processes provides the aperiodic, structured substrates from which natural selection can hone molecular information’.

The above leads naturally on to both the origin of life and Darwinian evolution.

11.3 Life’s emergence

In their mainstream biological text Life, Purves et al. ([8], pp. 450–457) explain three conditions that any model of emergence should satisfy: continuity, signature and no-free-lunch. The first means that any stage ‘should be derivable from pre-existing states’, the second that traces should be apparent in contemporary biochemistry, and thirdly, that sources of energy must be explicit. The extent to which this latter biology is viewed in the same way as our preceding thermodynamics is apparent from their ‘two long-term sources of free energy’, ‘radiation from the sun, and earth’s magma’, either or both of which ‘could have powered the origin of life’ ([8], p. 451).

Finally, Purves et al. make a telling point, that of economy: ‘biochemical evolution has been remarkably conservative’. This tends to resonate with Wicken’s rationale, which is that of economy of model. ‘One of the projects of this book’, he says ([10], p. 9), ‘will be to show that variation and selection emerged as evolutionary principles at the prebiotic level, and led to Darwin’s primordial organization. This extends rather than burdens the evolutionary project’, and below ‘... this
Table 4: What is life? — a synthesis of models.

<table>
<thead>
<tr>
<th>Model</th>
<th>Input</th>
<th>Activities</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Thermodynamics based</em></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Schrödinger [7]</td>
<td>Negative entropy</td>
<td>Avoids equilibrium</td>
<td>Heat rejection</td>
</tr>
<tr>
<td>Prigogine [7]</td>
<td>Free energy</td>
<td>(a) Far-from-equilibrium</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(b) Dissipative processes</td>
<td></td>
</tr>
<tr>
<td>Wicken [10]</td>
<td>Free energy (p. 36)</td>
<td>(a) Remote from equilibrium (p. 17)</td>
<td>Entropy (p. 31)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(b) Dissipative structures (p. 31)</td>
<td></td>
</tr>
<tr>
<td>Ji [36]</td>
<td>Free energy (pp. 5, 157)</td>
<td>Dissipative structures (p. 67)</td>
<td></td>
</tr>
<tr>
<td>Kauffman [50]</td>
<td>Free energy (p. 29)</td>
<td></td>
<td>Work cycle (pp. 8, 72)</td>
</tr>
<tr>
<td><em>Information based</em></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Schrödinger</td>
<td>Aperiodic solids</td>
<td>Autocatalytic system (pp. 17, 31)</td>
<td>Reproducing (p. 32)</td>
</tr>
<tr>
<td>Prigogine</td>
<td>Genetic constraints maintaining f–f–e</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wicken</td>
<td>Informed autocatalytic system (pp. 32)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AO organization</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ji</td>
<td>Shannon information (p. 1)</td>
<td>Autonomous agent (autocatalytic system) (pp. 8, 72)</td>
<td>Self-reproducing (p. 8)</td>
</tr>
<tr>
<td>Kauffman</td>
<td>Genetic material (p. 99)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AA autonomous agent</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

book … attempts to provide unifying principles for evolution …’. Such seems a commendable approach.

We conclude this entrée by noting Ji’s rather more speculative postulation based on the anthropic principle. It is that of the inevitability of life’s emergence, and the concomitant unity of cosmological and biological information ‘… the cosmological information encoded in the initial conditions of this planet at the time of the origin of life might have been necessary and sufficient to cause living systems to evolve spontaneously; i.e. these initial conditions might have acted as a ‘cosmological DNA’’. ([36], pp. 154/155). However, Ji’s ‘inevitability’ is mirrored both by Kauffman and by Wicken: ‘life is an expected, emergent property … autocatalytic sets of molecules suddenly become almost inevitable’ ([50], p. 35) and ‘The biosphere … necessarily provides niches in which AOs can emerge and evolve’ ([10], p. 117).

A detailed comparison is now made of the models for emergence of Wicken and Kauffman. Tables 5–8 compare respectively their overall strategy, salient features, the AO with AA and
Table 5: Comparison of emergence models of Wicken and Kauffman – (i) overall strategy.

<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td><strong>Darwinism</strong></td>
<td></td>
</tr>
<tr>
<td>(a) To discuss the structure that <em>allowed</em> crossing the bridge of autonomy that has isolated evolutionary theory from the physical sciences</td>
<td>(a) …order can arise without the benefit of natural selection…</td>
</tr>
<tr>
<td>(b) … a basis in physical law for the Darwinian principles of variation and selection</td>
<td>(b) Self-organization mingles with natural selection…</td>
</tr>
<tr>
<td>(c) To show how those laws … prebiotic evolution … conditions for life’s emergence (p. 131)</td>
<td>(c) We must, therefore, expand evolutionary theory (pp. 1, 2)</td>
</tr>
<tr>
<td><strong>Thermodynamics</strong></td>
<td>The emergence of a metabolism that solves the thermodynamic problem of driving the rapid synthesis of molecular species above their equilibrium concentrations (p. 47)</td>
</tr>
<tr>
<td>(a) Emergence is a systematic movement away from thermodynamic equilibrium</td>
<td></td>
</tr>
<tr>
<td>(b) The biosphere … necessarily provides niches in which AOs can emerge and evolve (pp. 116, 117)</td>
<td></td>
</tr>
</tbody>
</table>

Their triple-cycle autocatalysis concepts. It is important to include Ji’s triple-cycle model, the Princetonator, in the last comparison.

Table 5 shows that whereas Wicken has a conservatively Darwinian approach, Kauffman sees self-organization as an independent contributory factor in evolution. Despite this, in the context of their triple-cycle models, both see a *selective* drive. So for Kauffman, ‘Darwin’s natural selection could, in principle, operate if there were heritable variation in the kinetic constants’ ([50], p. 71). Wicken is emphatic. Summarising ([10], p. 131), he says ‘Selection was the central topic here’ in the whole emergence story. Table 5 also shows there is a common thermodynamic core, despite the latter being a problem for Kauffman, compared with a kind of driving force for Wicken. Table 6 again shows good agreement. Both disagree with the primal replication approach – ‘current life is not “nude” replicating DNA or RNA …’ ([50], p. 25), ‘less reasonable is the assumption … under the conditions of naked RNA competitions’ ([10], p. 103).

When it comes to hypercycles, Wicken classes them with the above problem, Kauffman accepting them. However, it is not completely clear whether Kauffman’s acceptance is for the *prebiotic* circumstances as well as later evolution. Then, it must be admitted that there is no reflection of ‘microspheres’ in Kauffman’s work, that is to say at the *equilibrium* level. Despite this, the end results of autocatalytic models (also see Table 7) and triple-cycle models (also see Table 8) are very similar. In Tables 7 and 8 material from Brooks and Wiley, and Ji are included, respectively.

In fact, the triple-cycle models of Wicken, Kauffman and Ji are strikingly coincident, and the conclusion must be that there is an underlying ‘commonwealth’ of thermodynamics. (A caveat must be that in constructing Table 8, it was not always clear that we could compare like with like). In fact, the authors’ descriptions show their commitment to a thermodynamic/biological synthesis.

Space does not allow further discussion of the still complex issues involved – for instance, Wicken (p. 128) – ‘we are still far from crossing the Kantian threshold to living matter. There are no *individuals* yet in this part of the epic …’.
Table 6: Comparison of emergence of Wicken and Kauffman – (ii) salient features.

<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Primal replication</td>
<td>Primal-replicator scenario paints itself into the … corner (p. 106)</td>
</tr>
<tr>
<td>Hypercycles of Eigen and Schuster [53]</td>
<td>… treating replicators as … primordial objects of selection imposes a need … in hypercyclic couplings – a need that defies the rules of selection (p. 101)</td>
</tr>
<tr>
<td>Alternative to primal replication</td>
<td>A more realistic possibility is that life emerged through … coevolution … within catalytic microspheres (p.106)</td>
</tr>
<tr>
<td>Microspheres</td>
<td>… is already a dynamic entity, capable of growth, chemical catalysis, and reproduction … (p. 124) … are equilibrium systems (p. 125) … this attempt to combine the best in the microsphere and hypercycle models (p. 110)</td>
</tr>
<tr>
<td>Autocatalytic systems</td>
<td>AOs (pp. 31–32, 17) figures 10-2 to 10-5 (pp. 127–128)</td>
</tr>
</tbody>
</table>

Table 7: Comparison of emergence models of Wicken and Kauffman – (iii) comparison of autocatalytic features, with references made by Brooks and Wiley.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Autocatalytic</td>
<td>✓ p. 31</td>
<td>✓ p. 72</td>
</tr>
<tr>
<td>Self-reproducing</td>
<td>✓ p. 32</td>
<td>✓ p. 8</td>
</tr>
<tr>
<td>Non-equilibrium</td>
<td>✓ pp. 116, 32</td>
<td>✓ p. 8</td>
</tr>
<tr>
<td>Dissipating structure</td>
<td>✓ pp. 74, 75</td>
<td>–</td>
</tr>
<tr>
<td>Expanding phase space</td>
<td>? the growth of microscopic information (p. 122)</td>
<td>✓ adjacent possible (p. 47)</td>
</tr>
<tr>
<td>Work output/energy storage</td>
<td>–</td>
<td>pp. 8, 72</td>
</tr>
<tr>
<td>Hydrophobic</td>
<td>✓ p. 126</td>
<td>–</td>
</tr>
</tbody>
</table>
Table 8: Comparison of emergence models of Wicken and Kauffman – (iv) comparison of triple cycle models, including the Princetonator.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Thermal cycle</td>
<td>Radiation in,</td>
<td>Photon source,</td>
<td>Solar radiation on</td>
</tr>
<tr>
<td></td>
<td>photoreceptor in</td>
<td>electron in</td>
<td>day–night cycle</td>
</tr>
<tr>
<td></td>
<td>x ground state</td>
<td>e ground state</td>
<td></td>
</tr>
<tr>
<td></td>
<td>x*excited state</td>
<td>e*excited state</td>
<td></td>
</tr>
<tr>
<td>2. Phosphate cycle</td>
<td>Yes</td>
<td>Yes (‘chemical engine’)</td>
<td>Yes</td>
</tr>
<tr>
<td>3. Replication cycle</td>
<td>T nucleic acid,</td>
<td>DNA hexamer,</td>
<td>A, B two kinds of biopolymers</td>
</tr>
<tr>
<td></td>
<td>N abiotic protein</td>
<td>plus 2 trimers</td>
<td></td>
</tr>
<tr>
<td></td>
<td>(see Quote W)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Notes: Authors’ descriptions.

Wicken: ‘… the fates of proteins and nucleic acids were bound together from the beginning – a primordial pair, yin to yang … the emergence of AOs based on their synergistic action was strongly selected for thermodynamically – and with it a translation mechanism. A minimal kinetic cycle based on these considerations is shown in figure 10-5’ ([10], p. 128).

Kauffman: ‘We measured efficiency thermodynamically as the conversion of available free energy coming into the system from the photon source into the excess hexamer, with respect to the undriven steady-state rate of reaction concentration of the hexamer’ ([50], p. 69).

Ji: ‘Clearly, the Princetonator provides a theoretically feasible molecular mechanism for biopolymer self-replication in the primordial soup that is driven solely by the solar radiation’ ([36], p. 225).

11.4 Thermodynamics and Darwinian evolution

11.4.1 The models of Brooks and Wiley, Ji, and Kauffman

11.4.1.1 Introduction We have pointed out that the model used by Brooks and Wiley appears to be divergent from the developed classical thermodynamics model of Wicken. In that context, Wicken’s approach may be regarded as conservative, both in his thermodynamics and his biology.

In this section we shall endeavour to show that: Brooks and Wiley’s model is redolent of a fundamental aspect of cosmological thermodynamics, reflected in the models developed by Ji and by Kauffman; what Brooks and Wiley term entropy might be replaced by, we suggest, a neutral as yet unquantified term, say ‘structure’; a reconciliation of the models of Brooks and Wiley and Wicken may be achieved by postulating the former’s ‘expanding phase space’ as a consequence of thermal driving forces, and that thereby their biological analyses are unaffected.

11.4.1.2 The model of Brooks and Wiley Underlying the entire rationale of Brooks and Wiley is the postulation that the second law of thermodynamics is but one manifestation of a more general ‘law of history’ (p. 356), and ‘entropy … a general manifestation of the passage of time indicated to an observer by time – dependent or irreversible, processes of all kinds (our italics).
All time-dependent processes, under this view, should exhibit entropic behaviour' (p. 355). So for Brooks and Wiley, the ‘second law of thermodynamics’ is replaced by the ‘(second) law of information’ and their entropy is no longer ‘thermal’ but ‘information capacity’ (pp. 71–73). For those (most?) of us who never found the thermodynamic entropy concept immediately digestible as were, say, heat, work and energy, this seems rather confusing, and Brooks and Wiley, again candidly, admit ‘their significant departure from classical thinking in thermodynamics’ (p. 52).

The outcome is expressed graphically by the generic model of Fig. 14. $H$ is the information-defined entropy, with $H_{\text{max}}$ the information capacity, ever increasing with time in consonance with cosmological expansion – in other words expanding phase space. $H_{\text{obs}}$ is the calculable Shannon information relevant to the specific biological application, termed complexity, as in Wicken’s suggestion. Brooks and Wiley use versions of this graph about 16 times throughout the book. In one application, that of phylogeny, the graph is quantitatively defined (figures 4.20 and 4.22, pp. 245/248). In this instance, time is defined as number of speciation events, and $H$ in bits of information.

Now, given the concept of increasing phase space (i.e. continuous expansion of the possible states a system can occupy) and ignoring the point that $H$ is claimed as an entropy, this approach gives an integrated and convincing description of the various strategic aspects of biological evolution. Moreover, the ‘adjacent possible’ concept of Kauffman ([50], p. 47), is completely consistent with this. Most radical is the ‘gnergy tetrahedron’ of Ji ([36], pp. 160, 231, 234). We have already noted Kauffman’s ‘concatenation of matter, energy, information, and something more that we call life’ ([50], p. 47). Ji combines just those items. ‘This line of thinking’ (that is of the ‘primeval substance of the universe’) ‘led me to postulate that the universe originated from gnergy, the primeval substance thought to be composed of a complementary … union of four essential entities, namely energy, matter, life and information. … I propose to use the term “energy–matter–life–information tetrahedrality of gnergy” to indicate the notion that gnergy is

Figure 14: Generic evolutionary model of Brooks and Wiley – the relationship between macroscopic information and complexity of a physical information system under the Brooks and Wiley theory (redrawn from figure 2.3 with title [25], p. 41).
neither energy nor life nor matter nor information but can manifest such properties or entities under the right set of physical conditions' ([36], p. 231). The energy tetrahedron is shown in Fig. 15.

Such multi-manifestations have, to us, too high an academic alcohol content. However, a much more dilute version, namely a possible direct energy to information conversion, is of considerable interest, and with this we retrace our steps. It is unquestionable mainstream thinking, as we have reviewed elsewhere, that the second law of thermodynamics is fundamental to the structure and history of the universe. It is also and equally accepted that due to cosmic expansion there is an entropy gap, which must be filled by thermal dissipation. In our case this is provided by solar radiation to us (of lower entropy) and then from us into space (of higher entropy). So the cosmic expansion effects are mediated to the earth thermally. Isn’t this just the grand ‘energetic imperative’ asked for by Brooks and Wiley ([25], p. 34)?

Now, in consistency with their model Brooks and Wiley postulate that in prebiotic evolution ‘monomer space’ microstates, then ‘polymer space’ become available ([25], p. 77). At face value this is correct, and an earlier publication by Kauffman is quoted in support. However, we have already seen that Kauffman himself makes the same point that we do, and in the context of prebiotic evolution “…there is an overall loss of free energy that is ultimately supplied by the incoming photon … plus the 2 substrates. … Thus, we are not cheating the second law” ([50], p. 57).

We can now suggest a holistic reconciliation of models, which only requires setting aside any need for other entropic laws. So Brooks and Wiley’s $H$-type entropy may be described in terms of order (‘structure’ is an as-yet unused example), and may properly express expanding phase space. This is now a consequence of free energy input to biological systems, and the Fig. 14

![Figure 15: The energy tetrahedron of Sungchal Ji (see figure 1.A5 [36], p. 234).](image-url)
type graphs, both encompass the biological applications and are consistent with the second law of thermodynamics.

11.4.2 An integrated survey of the work of Brooks and Wiley and of Wicken

…the reader may proceed to the summary of this chapter and then on to chapter 3, returning to the more technical parts of this chapter later.

Daniel Brooks and E.O. Wiley [29], p. 50
(referring to the 50 remaining pages of their ‘Core Hypothesis’)

The book in many ways is dense, both scientifically and philosophically. When encountering these densities…

Jeffrey Wicken, Preface [10], p. vi

It does not help the current authors’ case that these two key books, even after reconciliation, are not easy reading. They contrast, for example, with Kauffman’s publications in this regard. On the other hand, Brooks and Wiley and Wicken complement one another, the first being biologically oriented (‘… a unified theory … in biology’ ([29], p. 354)) and the second not (‘… little specific biology is discussed…’ ([10], p. vii)).

Much more important are their agendas related to natural selection.

For Brooks and Wiley ‘Current evolutionary thinking does not reconcile biological evolutionary theory with the four areas of contention discussed in this chapter. Such a reconciliation has not been reached because evolutionists have tended to focus on natural selection as the primary organizing factor in biological evolution. … We will attempt to develop … a theory of biological evolution that unifies the empirical core of neo-Darwinism … with these four major areas of “unfinished business”’, ([35], pp. 29, 30).

For Wicken ‘This book synthesizes a decade of my own work in extending the Darwinian program. … I think Darwin would have liked it. …’ ([10], p. v).

In both instances then, they constructively interact with natural selection. It is fortunate that both provide intermediate Summary sections, and presuming that readers wish to have direct acquaintance with their work, the following guide is given as Table 9.

Table 9: Identification of summary pages for understanding approaches of Wicken and of Brooks and Wiley.

<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>Part I – What is Life?</td>
<td>15/16</td>
<td>Preface</td>
<td>ix–xiv</td>
</tr>
<tr>
<td>Part II – Connection</td>
<td>53/54</td>
<td>1. Prelude</td>
<td>29/30</td>
</tr>
<tr>
<td>Part III – Emergence</td>
<td>95–97</td>
<td>2. The core hypothesis</td>
<td>102–107</td>
</tr>
<tr>
<td>Part IV – Biological evolution</td>
<td>131–134</td>
<td>3. Ontogeny, morphology and evolution</td>
<td>173–175</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5. Mapping historical change</td>
<td>287/288</td>
</tr>
<tr>
<td></td>
<td></td>
<td>6. Macroeocology</td>
<td>346–353</td>
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12 Conclusions

In this chapter an overview has been attempted of the relevance of thermodynamics to biology. Whereas the companion chapter in Volume 1 of the Design and Nature series focused primarily on energy, here the focus has been on entropy, information and complexity. It is shown that the concepts of free energy and exergy, which are equivalent and involve entropy, are necessary to a full understanding of engineering efficiency and to a thermodynamic model for living systems. It is demonstrated that, including thermodynamic variables, a mainstream interpretation of the evolution of the universe and the biosphere is emerging.

The relationship of entropy to information (Shannon entropy) and of both to complexity, are examined, and again a common interpretation is evident.

A number of authors have presented graphical models of the growth of information in the universe or the earth. These are compared, and again shown to be self-consistent. The concept of an ‘arrow of time’ of cosmic history is involved, and this stems from the second law of thermodynamics.

The key issues of what is meant by life, life’s emergence and of Darwinian evolution are reviewed, focusing on the comprehensive studies of Wicken, Kauffman, Sungchel Ji and of Brooks and Wiley. Comparisons of the various models are made in some detail, and display a convincing underlying unity. With the exception of Brooks and Wiley, the use of thermodynamics by all authors could be described as conservative. However, Brooks and Wiley’s model may be reconciled with the others by replacing their use of entropy with complexity, in the sense of consequential output, rather than input to living organisms.

The various authors include mathematicians, physicists, thermodynamicists and biologists. We conclude that their often very extensive studies point to a mainstream synthesis of biology and thermodynamics.

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References


