Some observations about the second law and life. Based on a dialogue with J.R. Minkel when he was writing the article on our work for *New Scientist*

By: James J. Kay © 2002

Why exergy instead of entropy?

Entropy is hard to get one's mind around because it is not a conserved quantity. Entropy is generated out of nothing when a process is irreversible. This entropy, which is generated, is not the total change in entropy in a process, as the process may also involve entropy changes due to the import or export of mass or energy. This nuance is often missed by people. There is also the issue of entropy generated and entropy change in the system and in the wider environment. It should also not be forgotten that one can only measure/calculate entropy change when a system changes between two or more equilibrium states. One CANNOT talk about the entropy of a system, only entropy change.

I have not seen a good general treatment of the relationship between entropy change, entropy generated in a system, and environment and exergy change. There are lots of examples of this being sorted out for specific cases, but not in general and not for biological systems (except for some specific cases). **This is the reason that dissipation and degradation are used in sloppy ways as it is never quite clear if one is talking about entropy change, entropy generation, exergy change, gradient change, or heat transfer and if it is for the system, or system plus environment.** We are working on this issue currently.

Bear in mind that thermodynamics is contemporary with quantum theory. Gibbs and Boltzmann's work were circa 1895 as was Planck's. Planck wrote the first text in thermodynamics. However over the past century, thermodynamics did not have nearly the brain power applied to it as did quantum theory. Thermodynamics is very much a science still in its very early stage of development. So the fact that there is a lot of conceptual murkiness should not be surprising.

"You said that entropy is only defined at equilibrium. so how can one talk about a system in which both exergy and entropy are changing at the same time?"

Yes this is a very tricky one.... Basically I can deal with entropy only in some special cases, for example steady state (even if not in equilibrium). For example in the Bénard cell, I cannot calculate the entropy generation in the cell directly. However I know that it is in a steady state, so the total entropy change must be zero and I can calculate the entropy change in the heat source and the cold sink, because they are in equilibrium, and the change in entropy of these must equal the entropy generated in the cell.

This is part of the reason I stick with exergy. I can calculate it in all situations without having to resort to various "tricks" and surrogates. Also if I try to talk about entropy production I don't know what the potential maximum is, whereas I know that the most exergy I can use is the amount I have. Also if I am using a certain amount of exergy relative to the exergy that there is, then I can define an efficiency of exergy use. There is no such equivalent for entropy.

Finally, from the point of view of a consumer, biological or otherwise, they see the exergy coming to them and can respond to that, they don't see the entropy they produce directly so they cannot respond to it directly. So from a self-organization perspective, it is not sensible to talk about entropy which the system cannot see, but rather about what it does with the exergy, which it can and does see.

The amount of entropy you produce, when you degrade a gradient, can change dramatically, depending on how the process used, degrades the gradient. Conversely you can create a specified amount of entropy by degrading different amounts of exergy or gradients. In other words, give me a gradient to degrade, and I can do it in a way which produces very different amounts of entropy. Gradient dissipation and exergy destruction simply do not track entropy production.

Exergy tells you about the theoretical limits on what you can do with the energy.

Entropy tells you how much irreversibility and uncertainty you produced in the way that you actually used the energy,

Exergy is about the potential to do something with the energy and entropy tells you something about what actually happened to the energy.

That is about as plain as I can say it in English without reverting to equations. When you look at the equations the difference between exergy and entropy is quite clear.

The reason I focus on exergy is that it is about how much out of equilibrium the situation is, how big the gradients are, and the potential to do something useful. For me these are the core issues. Entropy tells you nothing about these issues. It is not related to how big the gradients are, their potential to do something useful, or how out of equilibrium the situation is. It just tells you about the irreversibility that occurred in a process.

One trite but real difference between an exergy and entropy approach is this: If you talk about maximizing entropy, how do you know when you have gotten to the maximum? How can you test the hypothesis that entropy will be maximized? On the other hand you know when the gradient has been degraded (there is none left), when the exergy is gone (it is zero) and that you are in equilibrium. Furthermore if you have not gotten to equilibrium, gradients and exergy tell you how far you still have to go! A maximum entropy principle doesn't tell you how far you still have to go.

What is the relationship between exergy lost (i.e. degraded. destroyed) and entropy production?

"Why wouldn't you expect life to dissipate as much energy/make as much entropy as is possible even without the improved thermo? "

This misses the point or perhaps is THE POINT. Energy dissipation, entropy production and exergy use are not linked. You can use a lot of exergy, degrade a lot of exergy WITHOUT producing any entropy! You can produce lots of entropy without using any exergy! You can also dissipate a lot of energy without changing the exergy. The big step conceptually is to understand that entropy production, energy throughput or dissipation, and exergy use are three separate activities which are not necessarily related to each other. It is this separation which is why our ideas are so different from ones based on entropy production or energy dissipation. If you maximize entropy production or energy dissipation you get quite different phenomena from what we are suggesting..

The Gouy-Stodola theorem is a relationship between the lost exergy or exergy destroyed and the entropy generated. Basically the exergy destroyed is equal to the temperature of the environment (not the system) X the total entropy generated in the system and environment. The entropy generated is NOT the entropy change in a system, it is just the "new" entropy produced due to strictly internal irreversibilities. As Prigogine showed in his famous dS= dSe+dSi, you can have no TOTAL entropy change in a system if you import enough "negentropy" to offset the entropy generated. The exergy destroyed is only proportional to the entropy generated in the system and the environment.

Gouy-Stodola is about the total entropy change in the system + environment and I can talk about that often, but not always. Gouy-Stodola is limited to the special case when the system in only in contact with one environment at a fixed temperature. When radiation is involved as a means of energy exchange, then we are into a different situation. Also in the Bénard cell, there are two environments at different temperatures...... Gouy-Stodola doesn't apply in either situation.

"Some people claim that the law of maximum entropy production means that potentials/gradients will be minimized as fast and thoroughly as possible. Their definition of entropy seems to be increasing unavailability of energy to do work (not just heat energy), which still sounds like the inverse of exergy.

WRONG! People can try to define entropy anyway they want but in the end there is a technical and mathematical definition of entropy and exergy in thermodynamics and they are not related in this way

For a detailed discussion see:
http://www.jameskay.ca/musings/info.html

The important paragraph is:

> 'About useful information, exergy and entropy.
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> Given the above it is clear quite quickly why exergy and entropy are NOT opposites. EXERGY is the useful information we have about energy, gained when we transform energy from one form to another. ENTROPY increase is the uncertainty we have created about energy, when we transform energy from one form to another. They are not opposites for the same reasons stated above. So an increase in exergy occurs we gain more useful information about energy, that is we have more ability to do something with it. An increase in entropy corresponds to an increase in our uncertainty about energy. Work and heat are related by the first law and this makes them in a sense opposites but exergy and entropy are NOT conserved, one can change without the other changing. For example one can allow some exergy to "escape" from a system by letting it do work on its environment. By definition no entropy is produced! One can also construct systems where entropy changes without exergy changing. (Allow chemicals to combine and produce heat at the right temperatures and the loss of exergy in the chemicals is offset by the gain in exergy from the heat added to the system (i.e. the temperature increase).) This is why an entropy perspective on thermodynamics is NOT equivalent to an exergy perspective! One does need both to understand the second law dynamics of a system, just as one needs to consider useful information and uncertainty to have an "information theory". "

and the mathematical details in:
http://www.fes.uwaterloo.ca/u/jjkay/pubs/thesis/a1.pdf

As I said earlier, the amount of entropy you produce, when you degrade a gradient, can change dramatically depending on how the process used, degrades the gradient. Conversely you can create a specified amount of entropy by degrading different amounts of exergy or gradients. In other words, give me a gradient to degrade, and I can do it in a way which produces very different amounts of entropy. Gradient dissipation and exergy destruction simply do not track entropy production.

The long and the short of it is that there is no KNOWN general relationship between exergy lost and entropy produced[1]. All the ones we can find or produce ourselves are

[1] There does not exist a unique function F[entropy produced] such that for all situations: exergy lost = F[entropy produced].

special cases. I suspect that there is no general relationship between exergy lost and entropy produced. But I cannot provide a proof.

Thermodynamic Musings:
Three important things we realized:

1) The primitive in all discussions has to be gradient dissipation. Exergy loss, entropy production etc all being secondary effects. Gradients are the physical phenomena of nonequilibrium. Exergy is a common yardstick for measuring and comparing gradients in terms of the work that an observer can extract from different gradients under a common specific set of circumstances. Gradients are the phenomena and exergy a metric. Entropy is about how much disorder (irreversibility) is created when as a gradient is dissipated and the associated energy is converted to another form in the context of another gradient. As such it tells us very little directly about the gradient dissipation or what could be done with the gradient. It just tells us about the after effects of the gradient dissipation.

2) radiation is the most degraded form of energy, NOT HEAT. So the final step in any gradient dissipation process is radiation, heat being an intermediate stage.

3) Useful discussions of gradient dissipation must be in terms of several cascading gradients and thus hierarchical in nature. Anytime a gradient is dissipated it will result in energy transfer and hence the creation of a new gradient (unless you assume a spatially or temporally infinite reservoir as is usually done in classical thermodynamics, and we think it is this assumption which has blocked the development of a useful nonequilibrium thermodynamics.) So the question is how big and how useful is the new gradient and how far out of equilibrium are we now. (i.e. Are we any closer to equilibrium after dissipating the first gradient?) (Entropy cannot answer this question, only tell us how irreversible or disorderly the transition was.)

Probably it is quite unclear why theses things are important but they got us really excited and we think they provide a basis for much more useful discussions of nonequilibrium situations. [I think for the first time that we have come up with a framing for nonequilibrium thermodynamics.] They also suggest that discussions of entropy production, heat and thermal reservoirs are beside the point and it is focusing on them which has stood in the way of progress.

What do these ideas tell us?
It provides one with a sense that life WILL emerge and a sense of under what conditions. It provides me with a set of questions I would ask of a situation (and things to measure) to determine if life was likely to emerge. The point now is to determine the thresholds, like the Bénard cell thresholds. Right now we are working on developing such criteria and more importantly experiments to test them.

Our ideas also provide an explanation for some of the broad patterns of behaviour that we see in living systems, things like why are there lots of individuals instead of one big individual? Why is there a birth-growth-death cycle? Why is species diversity most strongly correlated with potential evapotranspiration? (We have the only explanation I know of.) Why do patterns like Hollings figure 8 on landscapes occur? In fact this is one phenomena that I have never seen a Darwinian explanation for, or any explanation, but I have provided an explanation which is experimentally testable! (See the CRC paper.) Why are ecosystems so inefficient at capturing solar energy and turning them into biomass? (If the point of life is to beget more life, then evolution didn't work out to well...... However from a thermodynamic perspective I would expect ecosystems to tend to be inefficient at converting solar energy to biomass, as they in fact are.)

We have only begun to tap into the possible concrete and testable predictions and insights possible.

Finally our ideas link life with other self-organizing phenomena in the physical world thus reconciling biology with physics and eliminating the need to treat biology as a special case exempt from the laws of physics.

Emergence of life

"Why doesn't life appear everywhere, if this idea is right? I'm pretty sure about the answer to that: you need sufficiently large gradients, something to carry information, nutrients, etc."

Exactly and not just sufficiently large, but not too large and there must be an appropriate match between the gradients, resources and information.

"NS ran a story about the RNA world in which Kauffman says that all you need for life to emerge is a certain collection of DNA, RNA, proteins, or whatever--some mishmash of life's building blocks--and they will spontaneously assemble into autocatalytic systems."

WRONG. The key ingredient is the gradients. You can have all the DNA and RNA you want and if there is not the appropriate gradient, nothing happens. On the other hand if there are gradients, you can bet that self-organization will occur and under the right conditions (with or without RNA, DNA etc) life will emerge.

Our version of thermodynamics goes one step further than just being consistent with the emergence of life, it mandates (demands) the emergence of self-organization and ultimately life. One has to appeal to nothing else to understand why life emerges! However the specifics of what kind of life emerges is a function of the details of the specific situation (and our theory tells you what details are important to consider!).

And furthermore what we are saying can then be used to generate testable hypotheses and be applied to real world issues like agricultural yield and fertilizer application. So our ideas go well beyond being academic curiosities.

Ecosystem Development

From: Ecosystems as Self-organizing Holarchic Open Systems : Narratives and the Second Law of Thermodynamics; Handbook of Ecosystem Theories and Management, CRC Press - Lewis Publishers. pp 135-160, 2000

> In examining the energetics of open systems, Kay and Schneider (Schneider and Kay, 1994a,b) noted that as an open system with exergy pumped into it is moved away from equilibrium. But nature resists movement away from equilibrium. **So in such a situation a system will organize itself so as to degrade the exergy as thoroughly as circumstances permit, thus limiting the degree to which the system is moved from thermodynamic equilibrium**. **When the input of the exergy and material pushes the system beyond a critical distance from equilibrium, the open system responds with the spontaneous emergence of new organized behaviour that uses the exergy to build, organize and maintain its structure.** This dissipates the ability of the exergy to move the system further away from equilibrium. As more exergy is pumped into a system, more organization emerges, in a step-wise way, to degrade the exergy. **Furthermore these systems tend to get better and better at "grabbing" resources and utilizing them to build more structure, thus enhancing their dissipating capability.** There is however, in principle, an upper limit to this organizational response. Beyond a critical distance from equilibrium, the organizational capacity of the system is overwhelmed and the system's behaviour leaves the domain of self-organization and becomes chaotic. As noted by Ulanowicz there is a "window of vitality", that is a minimum and maximum level in between which self-organization can occur.
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> The theory of non-equilibrium thermodynamics suggests that **the self-organization process in ecosystems proceeds in a way that: a) captures more resources (exergy and material); b) makes more effective use of the resources; c) builds more structure; d) enhances survivability (Kay, 1984, Kay and Schneider, 1992, Schneider and Kay, 1994a,b). These seem to be the kernel of the propensities of self-organization in ecosystems. How these propensities manifest themselves as morphogenetic causal loops is a**

function of the given environment (context) in which the ecosystem finds itself imbedded as well as the available materials, exergy and information.

From: Complexity and Thermodynamics:, Towards a New Ecology *Futures* **24** (6) August 1994

So as this discussion indicates, **we view ecosystems as the biotic, physical, and chemical components of nature acting together as nonequilibrium dissipative processes. The fundamental thermodynamic hypothesis about ecosystems is that they will organize themselves, in accordance with the second law, to increase the degradation of the exergy in incoming energy. A corollary is that material flow cycles will tend to be closed.** This is necessary to insure a continued supply of material for the energy degrading processes.

A second hypothesis, which is a consequence of the first, is that ecosystems will evolve and adapt so as to increase the potential for the ecosystem and its component systems to survive. Such behavior will assure the continued degradation of incoming energy. **This process is subject to the constraint that any evolutionary or adaptive strategy or mechanism which enhances survival is only economical if its net effect is to increase the energy degradation ability of the ecosystem. That is the thermodynamic cost (in terms of loss of loss of exergy capture capability) of the strategy or mechanism must be offset by the overall gain in energy degrading ability of the ecosystem.** Also, each component system will not be able to globally maximize its own survival because this would be done at the expense of other systems. Evolution and adaptation to improve survival potential are optimization processes subject to hierarchical thermodynamic and system constraints.

These hypothesis can be tested by observing the energetics of ecosystem development during the successional process, or by determining their behavior as they are stressed or their boundary conditions change. **As ecosystems develop or mature they should increase their total dissipation, and should develop more complex structures with greater diversity and more hierarchical levels to assist in energy degradation.** Successful species are those that funnel energy into their own production and reproduction and contribute to autocatalytic processes thereby increasing the total dissipation of the ecosystem. **In short, ecosystems develop in a way which systematically increases their ability to degrade the incoming solar energy.**

(Note This is an example of the aforementioned sloppiness in using the terms "dissipation" and "degradation". Opps! Dissipation means, as stated in the CRC quote, "dissipates the ability of the exergy to move the system further away from equilibrium")

Natural selection

"Is the idea that exergy degradation is selected for in the case of organisms?"

No it is not selected for in a neo-Darwinian sense, it is a generative principle, to use Wicken's term.

The evaluative principle is survival, subject to hierarchical constraints, of the individuals, the species and of the whole system. (Individuals who maximize their individual survival will always do it at the expense of the species as a whole and of the ecosystem. A species which maximizes its survival will do so at the expense of other species and the ecosystem as a whole (humans on earth right now!). So any criteria for maximization or minimization must be constrained by the bigger picture. This is the old system theory problem of suboptimization (A subsystem which runs optimally will cause the system to be suboptimal or reversed, subsystems must run in a suboptimal way in order to optimize the whole system.))

To quote from the 94 Futures paper;

> "As **ecosystems** develop or mature they should increase their total dissipation, and should develop more complex structures with greater diversity and more hierarchical levels to assist in energy degradation. Successful **species** are those that funnel energy into their own production and reproduction and contribute to autocatalytic processes thereby increasing the total dissipation of the ecosystem. In short, **ecosystems** develop in a way which systematically increases their ability to degrade the incoming solar energy."

From my thesis, ch. 2:

> "Component systems which share the same developmental pre-programming and are the largest physical units which individually spontaneously die (as versus death being necessarily the consequence of an environmental change) make up a class which will be referred to as a SPECIES. When an individual is referred to it is intended to represent the average adult member of the species. It is implicit that there is variability from one adult to another. Individuals need not be directly involved in the reproduction of the species, according to the above definition. The **individuals** are subject to the survival criteria (the last hypothesis above) as an evaluative principle. The **species** as a whole however is subject to the maximum degradation criteria... This maximization is constrained by the requirement that the **ecosystem** as a whole maximizes its degradation."

Note that the evaluative criteria for individual, species and ecosystems are DIFFERENT and I am referring to the SPECIES above NOT INDIVIDUALS. The hierarchical nature of these systems make things more complicated than simple minded neo-Darwinian survival of the fittest individual approach would lead you to believe. There is long discussion of this in Chapter 2 of my thesis

Also be careful that "capturing and degrading energy is selected for." even applied to individuals does not mean that they will be more efficient. You can be really good at capturing exergy and degrading it without being efficient. In fact forests are terribly inefficient in that they only capture and store 2% or less of the incoming solar energy, but they capture 85% of the incoming solar energy and degrade it (mostly by pumping water through the system). Things are not necessarily efficient at using the energy or exergy, they are just very efficient at capturing the exergy and destroying it.

In fact if we were to discover that specific organisms are very efficient at using the exergy, which means they capture the exergy and hold on to it, or they use the least amount of exergy possible to do a task, I would be willing to agree that the reason is, in their local circumstances, about natural selection and not a direct manifestation of the second law ALONE.

"I think the Darwinian could still argue that such behavior (things are not necessarily efficient at using the energy or exergy, they are just very efficient at capturing the exergy and destroying it.) leads to interactions between organisms that have survival benefits, so that behavior is selected for."

You are right about that. It is quite a challenge and I am no expert in Darwinian theory, so what follows in uninformed.

In specific cases certainly a Darwinian argument could be made but I am skeptical that it could be made in general. Our theory is general and predictive and my sense of Darwinian theory is that it explains things after the fact and Darwinian explanations are specific and not simple. Our ideas suggest a different way of thinking about evolution that leads to explanations of phenomena that are unexplained, and to asking different questions of the situation which lead one to collect different data. It leads you down a different path of inquiry.

And in some sense we get into tautological arguments. How would we disprove a Darwinian argument?

(It reminds me of the debate about Ptolemaic and Copernican world views. You could always add another epicycle to the Ptolemaic system to explain observations after the fact. It was not until Galileo, a hundred years later, looked at Venus through a telescope, that the issue was resolved.)

There is also the complication that we are not trying to negate natural selection. It is important. The point is that natural selection isn't enough to explain what we see happening by way of self-organization in living systems. A bottom up explanation like natural selection and cellular automata just are not sufficient to explain what is happening in complex systems because of emergent properties. Top down explanations based on general laws are also necessary. And a lot of people do not believe this. They believe that bottom up explanations are sufficient. This issue is not just about our theory versus neo-Darwinian theory but about systems theoretic explanations versus Newtonian mechanical explanations.

And frankly I have been surprised at how robust our predictions have been. I honestly expected that it would be hard to do experiments because the thermodynamic influence would be overwhelmed by the specifics of the situation, i.e. selection pressures in the local environment. So far it has turned out the thermodynamic influence produces a very strong signal which suggest that it is a very important component of evolution and self-organization.

But there certainly still needs to be thought and empirical work done to sort out the relative roles of natural selection and the second law.

That's all!