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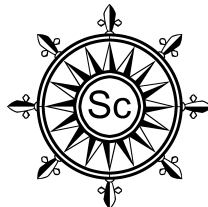
# Energy and Ecology

On entropy production and the analogy  
between fluid, climate and ecosystems

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# Abstract

We derive an expression for the entropy production (EP) of both phototrophic and chemotrophic ecosystems, and we apply this to simple models of generalized Lotka-Volterra ecosystems in a chemostat set-up in order to describe explicitly the coupling between the ecosystem and its environment. This allows us to determine the irreversibility of biological processes, whether the EP is an ecological goal function, whether the EP increases if a system is driven further out of equilibrium, and whether there are connections between EP and stability, competition, predation, biodiversity, efficiency or other hypothetical goal functions such as exergy. The EP as a candidate goal function also relates with the maximum entropy production (MaxEP) hypotheses applied in multiple physical systems, especially fluid and climate systems. We give a schematic classification of 11 different EP principles and hypotheses, as well as a criticism of some theoretical proofs of MaxEP that we encounter in the literature. We present an omnivore ecosystem as a counterexample for all MaxEP hypotheses in the non-linear response regime. We also formulate a practical definition of dissipative structures, and we apply this to ecosystems. Finally, we discuss an intriguing correspondence between ecosystems and fluid and climate systems. We demonstrate that the dynamical equations of a simple chemotrophic ecosystem correspond with the Lorenz equations for Rayleigh-Bénard convective fluid systems. Then we derive the size of convection cells by using an ecological competition principle. More generally, we postulate that the interactions of streams and whirls form a food web for the fluid or climate system.

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# Chapter 1

## General introduction

*Does it make sense to use a thermodynamic perspective on ecological processes?*  
*What do energy dissipation and gradient degradation mean for ecosystems?*  
*How to quantify the entropy production of ecological processes?*  
*Are biological processes more irreversible than abiotic ones?*  
*Are living states maximizing the production of entropy?*  
*Do ecosystems increase the entropy production when they are driven further out of thermodynamic equilibrium?*  
*How fast are non-equilibrium systems operating?*  
*How to define ecological goal functions, and do they exist?*  
*How to define dissipative structures?*  
*Are living organisms dissipative structures?*  
*Is there a correspondence between ecological systems and atmospheric or convective fluid systems?*

As the title 'Energy and Ecology' suggests, this thesis is situated in an interdisciplinary research combining the physical sciences with the ecological sciences. Energetic processes are studied in the physical science discipline called thermodynamics [88]. It is clear that energetic processes are also important in biology, the study of living organisms. Especially the molecular and sub-cellular levels lend themselves for thermodynamic studies. Increasing the scale of description - from the organism along the population towards the complete ecosystem - also increases the complexity. As ecology studies the interactions between living organisms and their interactions with their environment, one can focus on 'energetic' interactions. The latter are suitably studied in 'ecosystem ecology' [196]. Ecosystems are viewed as physical systems with energetic and material flows between different species, as the result of consumption (predation) relations. The flow network forms a food web (fig. 1.1) between different compartments (species). In recent decades, ecologists are trying to apply thermodynamics to ecosystems, forming a subfield of ecosystem ecology which is called *thermodynamic ecology*, and which studies the rates and efficiencies of energy transformations in food webs [81].

However, applying thermodynamics to bio- or ecological systems is not that straightforward. In the 19th century, two famous theories were introduced, and these theories were found difficult to reconcile with each other. On the one hand there is the theory of evolution and natural selection (survival of the fittest) by

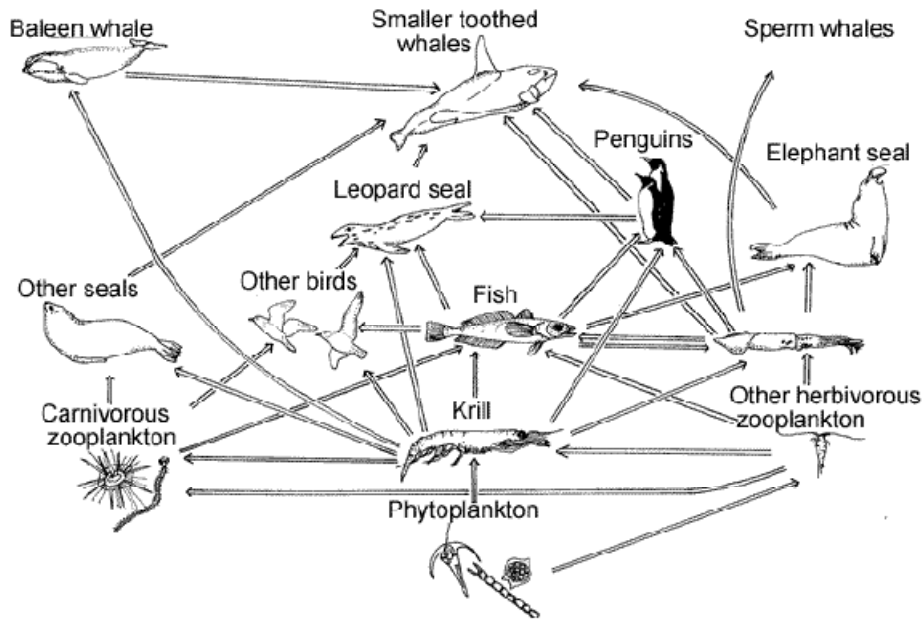


Figure 1.1: The Antarctic ocean foodweb.

Darwin in the biological sciences [44]. On the other hand we have (equilibrium or reversible) thermodynamics developed by Maxwell, Clausius, Boltzmann and others in the physical sciences. The latter resulted in the formulation of the famous second law which states that for closed and isolated systems there exists a measure of disorder, the entropy, that most likely increases when the system spontaneously evolves towards a state of maximum entropy, called the thermodynamic equilibrium. How does this relate to the development of living ecosystems, where evolution typically moves the ecosystem towards more order (less entropy) and ordered complexity? This gap between the biological and physical sciences, pointed out clearly by Boltzmann and Schrödinger [182], became one of the most basic questions in 20th (and 21th) century scientific research.

Briefly speaking, the solution of the above apparent paradox lies in the fact that firstly, ecosystems are *open systems*, not isolated ones. The total entropy of the universe should increase, but this is not in contradiction with a local decrease on earth. Secondly, the universe started *far from thermodynamic equilibrium*, with low entropy. This results into the fact that the sun is a low entropic object, radiating low entropic energy to the earth. This decreases the earth's entropy, and meanwhile all spontaneous processes on earth produce entropy which is emitted as high entropic radiation. Hence, understanding this ecosystem behavior requires non-equilibrium (or irreversible) thermodynamics for (energetically and/or materially) open systems. Not only ecological systems often develop towards "higher order". The same phenomenon might occur in purely physical systems that are open and far from equilibrium.

A prime example in physics where non-equilibrium thermodynamics becomes important is in the field of fluid dynamics, which has applications in atmo-

heric and climate systems. Take for instance the Rayleigh-Bénard system: A well studied system containing a horizontal viscous fluid layer which is heated from below. This heating, just like the sun's heating of the earth's surface, results in a temperature gradient that drives the fluid system out of thermodynamic equilibrium. When this heating is low, the fluid will simply conduct the heat upwards. But when the heating is large enough, a curious behavior appears. Suddenly, the fluid starts circling around in convection cells, an emergent coherent organization [14, 63, 162]. The uprising hot fluid motion increases the vertical heat transport. When cooled, the fluid moves downward to close the circulative motion. These so called Rayleigh-Bénard cells are structured in parallel rolls, hexagons or other ordered patterns. A similar behavior appears in atmospheric circulation, e.g. wind, hurricanes or large Hadley cells. These Hadley cells arise due to solar heating in the tropics, resulting into rising motion near the equator, a descending motion at the subtropics and equatorward flow near the surface. All these ordered fluid motions are 'laminar flows'. Increasing the heating further, the fluid system might reach a turbulent phase, with highly chaotic fluid motion [192]. The fundamental, unsolved problem in the field of fluid dynamics is how to characterize laminar versus turbulent fluid motion. More concretely: Why do these different types of motion appear only in specific parameter regimes (specific values for the heating)? How is the real state selected? How to understand the transitions from non-flow to laminar flow to turbulent flow when the fluid is driven further and further out of equilibrium? What is the microscopic origin of the ordered or chaotic macroscopic behavior? Can it be understood from first principles?

An interesting mathematical tool to understand a system (and perhaps to answer some of the above questions), which is used a lot in physics, is the *variational* or *extremal principle*. A quantity is varied with respect to one or more variables in order to find the maximum or minimum of that quantity. It is applied to find the state of a system and its stability [88], to describe fluctuations [105], to find dynamical laws, to find solutions of the equations of motion, to find constraints on the direction of processes and evolutions,... For example in mechanics, one has the Lagrangian or Hamiltonian formalism where the principle of least action is used to find the equations of motion [170].

Extremal principles are also fruitful in thermodynamics. The best known example is the above mentioned second law of thermodynamics. The macroscopic dynamics of a system is restricted because the entropy should increase. Thermodynamic equilibrium can be found by maximizing the entropy. To understand the notion of entropy at a more fundamental level, one has to look at statistical mechanics. In thermodynamics, a system is described by a macroscopic state, with macroscopic variables. But the same macroscopic state can be realized by different microscopic states. The entropy is a state function which basically counts the number of microscopic states compatible with the same macroscopic state. Hence, from a statistical point of view, supposing that every microscopic state has the same probability, the system is most likely to be found in equilibrium, because that macroscopic state has the most microscopic states (i.e. highest entropy). Understanding this idea was a great improvement for equilibrium thermodynamics.

For non-equilibrium thermodynamics, the situation is much more complex. Close to equilibrium, it was shown by Prigogine and others (see e.g. [88]) that

one does not have to look at the entropy, but at the entropy production (EP)<sup>1</sup>. If a system is open, and the environment with which it is coupled drives the system slightly out of equilibrium, the steady state of the system can be found by minimizing the EP (MinEP). No extremal principle far from equilibrium is known to exist. Nevertheless, there are various arguments to study the behavior of the EP for systems in the far from equilibrium regime.

1) Total EP is the time derivative of the total entropy of system plus environment. It combines the basic notion in thermodynamics, entropy, with the basic notion in non-equilibrium dynamics, time. Dynamic non-equilibrium systems involve transitions in a finite amount of time. Therefore, one is forced to abandon the traditional picture of an ideal heat engine of the Carnot type and one should incorporate dissipation in the description. Dissipation is the turn-over of available (qualitative) energy (the energy that can perform work) into unavailable (useless) energy. In the formalism of irreversible thermodynamics, the dissipation is given by the EP. The EP is the most natural measure for irreversibility.

2) By studying the EP as a natural measure for irreversibility, one can try to find relations with e.g. the second law (positivity of the EP). As EP measures the loss of available energy, it is related with the important notion of thermodynamic efficiency.

3) In its mathematical expression (which we will derive in later chapters), the EP is written as the product (a bilinear form) of thermodynamic forces and fluxes. Philosophically speaking, the forces are the causes and the fluxes are the effects. The forces measure how far the system is out of equilibrium. They are analogous with e.g. the steepness of a river. The fluxes (of particles, heat, energy,...) measure the systems response to the forces. They are analogous with e.g. the flow velocity of the river. As the EP can be written as the bilinear form of causes and effects, and therefore "unifies" causes and effects, it is a mathematically elegant quantity to study the system behavior.

4) Recent decades show a revival of the EP as a candidate for an extremal principle. Especially the literature on the maximum entropy production (MaxEP) hypothesis is growing [86, 110, 148], with an increasing amount of experimental corroboration. There are different formulations of the MaxEP hypothesis, but roughly speaking it claims that (under some constraints and conditions) the selected state of the system is the one with highest EP.

5) As mentioned above, ordered patterns might appear in fluid systems driven far from equilibrium. Similar kind of spatially or temporally ordered patterns arise in many other physical non-equilibrium systems, like chemical reaction systems. Prigogine and co-workers [65, 88, 134] termed these systems 'dissipative systems', and the resulting patterns 'dissipative structures'. Close to thermodynamic equilibrium these structures are unstable and they decay, because they have lower entropy than the unstructured state. But far enough from equilibrium, spontaneous fluctuations might grow into stable structures with low entropy. These structures maintain themselves by dissipating energy, i.e. taking up low entropic energy from the environment, and emitting high entropic energy. It is believed that this dissipation, i.e. the EP, is crucial for a good understanding of these systems. Furthermore, as hinted at by Schrödinger [182]

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<sup>1</sup>In our terminology, the EP is always assumed to be a 'rate' (with units Joule per Kelvin per second), but the latter word will be omitted for simplicity.

and Nicolis and Prigogine [134] living structures are believed to be dissipative structures.

The latter brings us automatically to the fields of biology and more specifically ecology. Living systems are viewed as thermodynamically open, far-from-equilibrium systems. From a non-equilibrium thermodynamic point of view, the environment is highly important, because as we have seen, they can drive the system out of equilibrium by applying thermodynamic forces. As in far-from-equilibrium fluid physics, also bio- and ecology have a basic question: *What characterizes life?* More concretely: Why does life appear? How do organisms and ecosystems evolve? Amongst the vast amount of studies, one specific direction of research was the integration of thermodynamics and statistical mechanics with biology and ecology [81]. The search towards correct formulations of the existence of thermodynamical constraints in bio- and ecosystems is still ongoing, because when looking at an ecosystem as a large, open chemical reaction system, one has to take into account not only thermodynamic, but also kinetic constraints [160], involving multiple feedback mechanisms, making the problem very complex. This search for thermodynamical constraints and linking the science of ecology with the laws of thermodynamics is part of the more general search for underlying organizational principles of ecology. And perhaps a reconciliation of (biological) self-organizing systems and thermodynamics might yield new principles of physics as well.

Some of these studies in thermodynamic ecology (or 'ecological thermodynamics') try to understand evolution from a thermodynamic perspective (e.g. is evolution - which is typically irreversible - a consequence of thermodynamic irreversibility?) [19, 23, 55, 64], often at the philosophical level [204, 206]. Others are studying the metabolism of organisms, trying to explain so called scaling laws (e.g. power law relations between the respiration rates and the sizes of organisms) from a thermodynamic perspective [24]. The latter approach led some researchers to the 'dynamic energy budget' theory [187]. Some use information theory [41], others focus at the thermodynamic efficiency of ecological functioning [39] or make the link between thermodynamic ecology and economics [40, 168]. But there is one line of research in the theoretical ecology literature that is of specific interest to us: the search for variational (extremal) principles, which the ecologists have termed ecological goal functions or indicators.

Due to processes like speciation, immigration, species interactions, competition and many others, ecosystems (sometimes or often) evolve towards a so called climax state, a state which is highly stable against perturbations (see [196] for a (critical) discussion). From the ecosystem point of view, one is interested in the evolution of the food web and its properties in the climax state. In order to describe ecosystem evolution, researchers introduced the notion of a goal function. These goal functions are the basic quantities of organizational principles, very similar to the extremal principles used in physics. Just as the entropy of an isolated system spontaneously increases towards a maximum, it is hoped that some ecological quantity exists which spontaneously increases (or decreases) towards an optimal value. Some of these ideas are already quite old. The first proposal was done by Lotka [99], claiming that energy throughflow increases. A second proposal was made by Margalef [109], taking the total biomass instead of the energy throughflow as the goal function. In recent decades, there has been an increase of studies involving goal functions, especially in the ecological modeling discipline, to find the selected or most probable state of an

ecosystem.

It is believed that the possible existence of goal functions might shed some light at the stability-complexity debate. This debate in the ecology literature started by the work of May [113]. It was generally believed that a complex (e.g. a biodiverse) ecosystem is more stable than a simple ecosystem. But May demonstrated that an ecosystem that is constructed 'randomly' (i.e. the interaction strengths between

the species are chosen randomly) becomes less stable when the complexity (biodiversity) increases. Obviously, natural food webs are not 'random', but the interaction strengths are somehow constrained [115]. Some ecologists share the hope that an organizational principle such as a goal function might explain the constrained properties of stable food webs. And as species are believed to evolve to new species which are more efficient in e.g. capturing and using free energy, there might also be relations between goal functions and (thermodynamic) efficiency. These relations might determine the overall ecosystem food web structure.

Another reason why goal functions became important is that some ecologists hope that they can help monitoring the maturity of ecosystems. How do we know that an ecosystem is functioning optimally? Can we see when an ecosystem is 'disturbed'? Consider for example the human body. It has a highly non-trivial and very useful property. Due to its endothermic (warm-blooded) self-regulation, the human body functions optimally at the temperature of  $37^{\circ}C$ . Complex feedback mechanisms try to regulate the temperature, and the 'goal' of this regulation is the optimal temperature. Furthermore, when the body has fever, we say that it is ill. What makes this temperature quantity particularly interesting is that we have equipment to measure it. Some ecologists dream to find an analogous quantity, not for an endothermic body, but for a whole ecosystem.

And a third motivation to look for goal functions is the hope to find some emergent properties. As ecosystems are very complex, one might ask the question whether it is really necessary to study every organism and consider every interaction in order to understand ecosystem functioning. As thermodynamics and statistical mechanics shows, it is possible to derive non-trivial global properties of a gas of many particles, even though microscopic states and interactions are unknown. The hope is that there is some emergent ecological property when we study the ecosystem at a large scale. Can we take a 'thermodynamic limit', use a statistical law of large numbers, for ecosystems with many species ('many degrees of freedom'). And furthermore, would the emerging property resemble a goal function?

We are now beginning to see a common ground between physical and ecological sciences, between extremal principles applied in physics (thermodynamics) and goal functions in ecology. We have met three examples that showed that the goal function idea is not that far fetched:

- 1) For an isolated system we can see whether it is disturbed from thermodynamic equilibrium by looking at the entropy. The entropy is maximal in the undisturbed equilibrium state. Maximum entropy is the 'goal'.
- 2) For open systems close to equilibrium the thermodynamic EP can be used to see disturbances from the steady state. As mentioned above, Prigogine discovered that minimum EP is the 'goal'.
- 3) For the human body, the temperature of  $37^{\circ}C$  ( $310K$ ) is a target value. A

disturbance ('illness') results in a deviation.

So the question is: Do ecosystems as a whole have an analogous 'disturbance' or 'illness' measure? And if the answer is 'yes', can we easily measure it? Some goal function proposals depend only on ecological variables and parameters (e.g. biomass, productivity, growth rates,...). But the successes in thermodynamics (note that in the three above examples, the entropy, the EP and the temperature are all thermodynamic concepts) lead a lot of ecologists to studying thermodynamic goal functions [79, 81]. This lead to land-use-impact studies by monitoring e.g. the ecosystem temperature [3, 202]. Candidates of thermodynamic ecological goal functions have names like e.g. exergy [80], emergy [140] or ascendancy [198]. But also dissipation or entropy production [6, 101, 179] was proposed as a goal function.

This moves us finally back to physics. In the attempt to answer questions like: "How fast are non-equilibrium systems operating?" and "How efficient are they?", both physicists studying far-from-equilibrium systems (e.g. fluid or climate systems) and ecologists are now looking for thermodynamic organizational principles, especially in terms of extremal principles and ecological goal functions. And as both fluid and ecological systems are believed to be dissipative systems, the monitoring of the dissipation, measured by the EP, might perhaps lead to interesting results. It is hoped that thermodynamic ecological goal functions might explain a lot of phenomenological relations and observations, like e.g. efficiencies in energetic transfers, constraints on the length of trophic food-chains or the flows between biological and environmental compartments.

Applying thermodynamics to ecosystems not only involves studying thermodynamic goal functions. Even if goal function candidates such as the EP are not evolving towards an extremum under ecosystem development, one can still try to look for correspondences between physical and ecological systems. In fact, there are some intriguing and highly non-trivial analogies between the above mentioned Rayleigh-Bénard convective fluid systems, climate systems and ecosystems.

## 1.1 Overview thesis

Roughly speaking, this thesis contains three contributions. A bit exaggerated, we will first prepare some rigid foundations (chapters 2 and 3). These foundations make us strong enough for our second operation: a 'demolition' of weak theories and hypotheses (chapters 4 till 8). After the breakdown, we want to end with a positive story. We will build up stronger constructions (chapters 9 and 10). In particular, we will build a beautiful bridge...

Chapter 2 will present the fundamental problems in thermodynamic ecology. There are four basic questions: What is the correct choice of variables? How to measure the entropy of organisms? How to distinguish between ecosystem and environment? And how to determine the steady state? These problems have to be tackled when we study and derive a reliable expression of the ecosystem EP. Our starting point is classical irreversible thermodynamics [88], in particular chemical thermodynamics in local equilibrium systems [47]<sup>2</sup>. Our approach

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<sup>2</sup>We will not study statistical mechanical aspects of EP in this work [89]. Some aspects in the field of non-equilibrium statistical mechanics were studied in [217, 218].

also clarifies some limitations of the use of the EP as a quantity that characterizes systems far from equilibrium. In order to avoid the basic difficulties in thermodynamic ecology, we will systematically apply simplifications in order to arrive at expressions for the total EP in the steady state. This quantity is simple enough to be well defined, but complex enough to have non-trivial behavior. Model universes for both chemical reaction systems (in terms of a laboratory chemostat set-up) and radiation systems (in terms of a planetary radiation balance) will be presented, with a special emphasis on the coupling between system and environment. These two general models serve as very basic descriptions of resp. *chemotrophic* and *phototrophic ecosystems* (see appendix A for a glossary of some terminology). The former contain organisms feeding on a chemical energy substrate, whereas the latter systems contain organisms that take up radiation energy by photosynthesis. A highly important conclusion is that thermodynamic ecology has to look not only at the ecosystem, but also at the exchanges with the environment. The environment has different reservoirs, containing resource at high energetic quality, or waste products at low energetic quality. This energetic quality difference means that the environmental reservoirs are not in mutual (global) thermodynamic equilibrium, and it is this non-equilibrium which is crucial. It drives the resource processing, the growth of organisms, the development of complex food webs. In short, it drives the ecosystem metabolism. If we could study the EP of this fundamental ecological quantity...

Chapter 3 gives a more detailed presentation on the chemotrophic ecosystem<sup>3</sup>. The ecosystem is treated as a 'black box', but a rough description of the basic internal processes is given. This allows us to focus on the ecosystem metabolism, and the way how it depends on the food web through an 'effective' rate parameter that measures the timescale of the resource processing within the ecosystem. Plotting the steady state EP of the ecosystem metabolism as a function of this parameter, we can see that the EP goes through a maximum when the rate parameter increases. The natural question is whether realistic ecosystems have a resource processing rate close to this maximum value. This will be our first encounter with the ecological goal function hypothesis, and also with the maximum entropy production (MaxEP) hypothesis used for e.g. the global heat transport in the earth's climate system. Both ideas have some intriguing similarities. Hence, two recent and growing fields of research (entropy production in ecology and in climatology) will be meet each other. After having derived a rigorous EP expression, we can compare our result with other studies...

Chapter 4 is the start of our second and biggest task: the 'cleaning of the Augeas stable'. A large amount of criticism is given to various approaches and ideas in the literature. Chapter 2 focussed at the EP for *general chemical reaction systems in a 'very black box' fashion*. Chapter 3 did the same job, but add a little more color to the black box by studying the basal functioning of *chemotrophic ecosystems*. In chapter 4 we go again one step further. By studying a more specific dynamics of competitive and predatory interactions, we will add yet more color to the models of the chemotrophic ecosystems of chapter 3, and turn them into an important type of chemotrophic models: the *generalized*

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<sup>3</sup>This chapter is based on the article [219]. As it is written in a self-contained way, it can be read independently.

*Lotka-Volterra chemostat ecosystems* [30]. These models have a coupled set of non-linear ordinary differential equations, whereby the biomasses (or the concentrations) of the species are treated as continuous variables. When the EP is studied in a quantitative way in the literature, it is typically applied to Lotka-Volterra systems. Therefore, the focus of chapter 4 lies on the discussion of some expressions for the EP for Lotka-Volterra systems. We will demonstrate that these expressions are either wrong or only valid in a very restricted sense. To avoid confusion, some of the quantities in those studies should be given other names. The criticism on those EP expressions is in clear contrast with our approach, which is much more reliable.

Excluding other EP approaches is one thing, but this does not end the job. We have to look at the studies that use the correct expression for the EP, but still create confusion. What is more, in this chapter we encounter a second MaxEP hypothesis, which is unrelated with the MaxEP in chapter 3. But MaxEP does not stop with only two different hypotheses...

Chapter 5 claims that there is more confusion in the literature, not only the thermodynamic ecology literature, but a much larger field of research, including physical systems such as chemical reaction, electrical, fluid or climate systems. We delve deeply in

the MaxEP discussion. But we have to be careful in this often confusing MaxEP area: After a vast research of the literature, we can conclude that there are no less than 11(!) different EP proposals. What is more: not a single article was found that clearly points at the differences between some MaxEP's. So our next task is to study the differences (and similarities) between the MaxEP's. This can only be done by a systematic classification in order to disentangle the knots. Having set-up the classification allows us to more rigorously define all the EP hypotheses. After these formulations, we have to look for proofs. As it is not directly relevant for ecology, we refer to the article [217], which contains a discussion and some more comments about a few theoretical proofs for MaxEP hypotheses with techniques borrowed from statistical mechanics and information theory. To summarize that article, a simple stochastic non-equilibrium physical toy model is presented, that models particle fluxes in a network. The remarkable but useful property is that this model is mathematically equivalent with an equilibrium ferromagnet model. The new point of view is that the former non-equilibrium system looks at the path space, whereas the latter is an equilibrium system that typically considers the microscopic state space. As the latter model has simple expressions for e.g. the mean magnetization, this equivalence allows to write down simple expressions for e.g. the average fluxes and the EP in the non-equilibrium system. The reader who is not interested in technicalities might skip this chapter, because the ecological relevance is rather low and the conclusion is very simple: The discussed proofs are unsatisfactory or incomplete. If proofs are absent, then perhaps we have to look for counterexamples...

Chapter 6 moves us back to ecology, for it discusses a theoretical resource-consumer-omnivore (RCO) system as a specific generalized Lotka-Volterra chemostat ecosystem. This one model is quite strong, as it will serve as a counterexample to basically all interesting (non-linear response) MaxEP hypotheses discussed in chapter 5. Questions like 'Is the most stable steady state also the one with the highest EP?' and 'Does the EP increase when the system is driven further out of equilibrium?' will be answered in the negative. We will also discuss some proposed relations between the trio EP, ecosystem stability

and biodiversity, and here again the results are quite disappointing. Up to this point, the only rule for the EP behavior is that 'anything goes' (except that the EP for every independent irreversible process should be positive). If EP is not such a nice candidate for goal functions, perhaps we have to look at other goal function proposals...

Chapter 7 discusses ecological goal functions and the possible links with efficiency measures and evolutionary fitness. This requires first of all that we define a goal function, because the literature does not offer us a precise notion. We will give three possible definitions. Next, some specific candidates for a goal function need to be defined for a specific system. We will use a theoretical resource-consumer-predator (RCP) system as a specific generalized Lotka Volterra chemostat system. But here we encounter problems mentioned in chapter 2. In order to deal with them, some explicit (and perhaps highly unrealistic) assumptions have to be made. the ecosystem will be approached as a chemical reaction system in local equilibrium. This allows for explicit expressions of all the kinetic and thermodynamic quantities, but treating organisms as ideal solutions might be far fetched. However, brave as we are, we stick to this simplified ecosystem model. We continue with presenting a huge list of goal function proposals ever made in the literature. This involves e.g. an alternative derivation of an important candidate goal function, the exergy, with new interpretations of the terms in the exergy expression. (We refer to [223] for a review on exergy in environmental sciences and technology.) All of these goal function candidates will consequently be tested according to the three definitions. We also look for possible correlations in behavior. E.g. are organisms that are more efficient in using free energy also evolutionarily stronger? Does that also lead to a gradual increase of free energy degradation (EP) or energy throughflow under evolution? Does that mean that efficiency is correlated with EP under evolution? In our search, no non-trivial relations were found however. None of the goal function proposals obey any of the three goal function definitions in a non-trivial way. Perhaps our model is too simple. Or perhaps the goal function definitions are too restrictive, too strong. There is a much 'weaker' question regarding the EP of life, related with the definition of dissipative structures...

Chapter 8 discusses the possibility for ecosystems (as well as fluid and climate systems) to contain 'dissipative structures'. Similar to the chapter 7, we first have to define what we mean by this notion which is left quite vague in the literature. Therefore, with the help of the study of Rayleigh-Bénard convection systems, a simple and practical definition for a dissipative structure is given, containing only two requirements. The first is the existence of non-trivial bifurcation points for the thermodynamic gradient. For values below this critical level, no structures are sustained, but when the gradient passes beyond the bifurcation point, the structures appear. But the second requirement is more intriguing. The goal function definition required that e.g. the EP is *maximal* in the selected steady state. The dissipative structure definition is weaker, it only requires that the EP is *higher*. More specifically, the steady state of a system with stable dissipative structures should have more EP (synonymous with 'dissipation') than the unstable unstructured steady state at the same boundary conditions (e.g. the same external gradient). We call this requirement 'ultra dissipation'. Translated to biology, it asks the question: "Does life increase the EP?", in other words: "Are living processes 'more irreversible' than abiotic processes?" or "Does a living state have a higher EP than the dead state at

the same boundary conditions?” All our models (the RCO and RCP) discussed in previous chapters were nice counterexamples for specific hypotheses such as MaxEP, because they had analytical solutions (no numerical simulations as in [130, 31, 184] required) and the EP could be calculated arbitrarily far from equilibrium<sup>4</sup>. But calculating the EP of the biotic state, it was always found to be higher than the dead state. In other words, the biotic state was always ‘ultra dissipative’. In order to study this subject more rigorously, two models are constructed, a chemotrophic and a phototrophic. The latter can also be applied to the earth as a whole, because it allows to study the radiation balance of the earth climate. These two models have one global physical variable (the average resource concentration and the average temperature resp.) and one global biotic variable (the average consumer concentration and the fraction of land cover)<sup>5</sup>. Both models show an ‘infra dissipative’ behavior, whereby the living state has a lower EP than the dead state at the same boundary conditions. We can conclude that for this theoretical description, there are no indications that life should always increase the EP. A lowering is also possible and for these situations the living biota would be ‘anti-dissipative structures’.

Here ends the cleaning of the Augeas stable (or stables). Theoretical studies show that a lot of proposals do not work. Cleaning up (or rather ‘breaking down’) ideas is one thing, which is sometimes necessary in critical scientific research. But coming up with a positive, constructive story is something else...

Chapter 9 is the bright peak of our research. Therefore, we have written it in a self-contained manner, such that it can be read independently from the other chapters. It presents an intriguing idea that is so challenging, that it might set up a new research program. The key point is that we might have discovered a ‘Rosetta Stone’ between physical systems, in particular Rayleigh-Bénard convective fluid systems, and ecosystems, in particular resource-consumer (RC) chemostat systems. A simplified description of the convective fluid system has been studied by climatologist Lorenz [97], which resulted in a set of three ordinary differential equations, the XYZ model. These equations became famous for its property of deterministic chaos. The remarkable discovery is that a specific formulation of the dynamics, the quasi steady state Lorenz dynamics (the XZ model), can be rewritten in such a way that it exactly resembles the RC ecosystem dynamics. For example the kinetic energy of the convection cells turns out to be equivalent with the biomass concentration of the consumer, and heat convection is similar to biotic resource conversion. As a practical consequence, we can include competition, which will lead us to an alternative derivation (different from Rayleigh in [162]) for the value of the size of the convection rolls. Can one also include predation? We conjecture that the resource-consumer-predator (RCP) system is analogous to the fluid system with wavy convection rolls. But the quasi steady state Lorenz dynamics is a crude approximation of the full Lorenz system (the XYZ model)...

Chapter 10 first studies the translation of the full Lorenz dynamics to an

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<sup>4</sup>‘Arbitrarily far’ should not be taken too literally. We can calculate the EP also beyond higher bifurcation points, in contrast with e.g. [179] where only the EP around the first bifurcation was studied. But eventually our description has its limits, as the classical irreversible thermodynamics formalism, based on local equilibrium, might fail very far from equilibrium.

<sup>5</sup>The homogeneity (averaging) of our description does not allow us to measure spatial properties of the structures, but our definition remains applicable. Therefore, our definition avoids difficulties relating with the measurement of the ‘ordered complexity’ of the structures.

ecological system. The answer might be in the affirmative, as we present a limiting case of a model for biological cell growth which is mathematically equivalent with the XYZ model. We conclude the chapter with further speculations and open questions. Is the earth atmosphere (with predation and competition between different wind flows, hurricanes, eddy currents,...) similar to an ecosystem with a complex food web? Is there 'evolution' in the patterns formed by Rayleigh-Bénard convection cells? Is there a new hope for the MaxEP hypothesis encountered in chapter 3, after giving it a strong blow in chapter 6? Are the underlying microscopic mechanisms (the information transfers,...) also similar in both fluid and ecosystems? It appears that we can build a beautiful bridge between two scientific worlds, the world of physics (in particular the thermodynamics of fluid and climate systems) on the one side, and the world of ecology on the other. We end with some highly speculative philosophy, by asking the question: "What is life, if its functioning seems to be so similar to fluid and climate systems?"

As an endnote, we conclude this work with a personal confession/opinion about the performed interdisciplinary scientific research and the general status of the field of thermodynamic ecology. One of the major difficulties in interdisciplinary research is that different branches of sciences (especially physics and ecology) have different languages. Along our road, we will encounter radiation physics, fluid physics, non-equilibrium thermodynamics, statistical mechanics, information theory, nonlinear physics, atmospheric physics, climatology, chemistry, biology, population ecology and ecosystem (food web) ecology. Therefore, some concepts might be unfamiliar to the reader. Appendix A contains a glossary of some important terms, and for the ones who are confused with the notation, appendix B might be of some help.

## 1.2 The most important results

Let us summarize the most intriguing, 'tasty' results of our research. Perhaps these results can be best summarized by the statement: *There is a correspondence at different scales of complexity between physics, in particular heat transport in fluid and climate systems, and ecology, in particular ecosystem operation.* Fig. 1.2 shows this basic correspondence, our scientific 'Rosetta Stone'.

At the most complex level of description, the 'megascopic' scale, there is an analogy between e.g. the earth climate system with multiple types of fluid motion (large Hadley cells, hurricanes, smaller eddies,...) on the one hand and a complex ecosystem such as the sediment at the ocean floor or a chemostat with multiple species (bacteria, ciliates, copepods,...), on the other, see fig. 1.3.

Both the earth and the sediment ecosystem have an input of energy of high quality, be it high temperature (high frequency) heat radiation or organic (reduced) resource compounds. This high quality energy is processed by the system into waste products at low energetic quality, e.g. low temperature radiation or oxidized  $CO_2$ , and this waste energy is emitted to a background environment. For the earth atmosphere, the energy processing is done by conductive and convective heat transport from the tropics to the poles. Similarly, the sediment has an ecosystem metabolism: the biota are degrading (oxidizing) the resource (the food). In the figure, this energy processing is indicated with arrows with fat contours, because they are the most important.

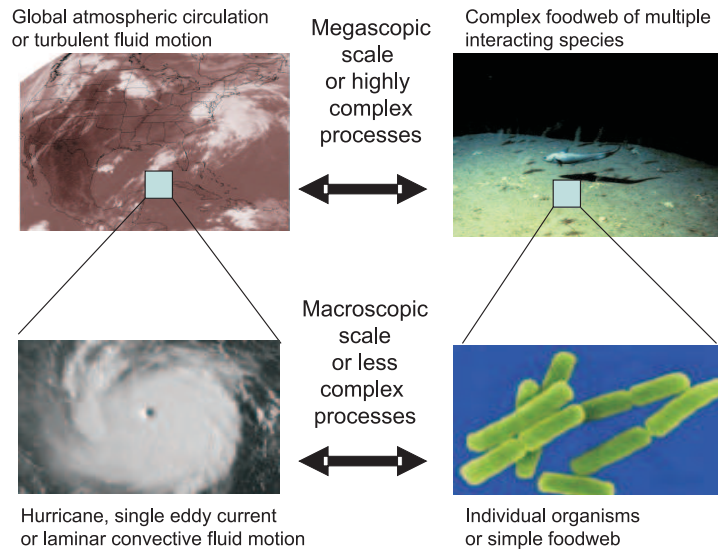


Figure 1.2: The correspondence between fluid/climate systems and ecosystems at different levels of complexity. A complex fluid system at a 'megascopic' scale might correspond with a complex fluid system. At a macroscopic scale, a single population of organisms might corresponds with a specific type of patterned laminar fluid motion.

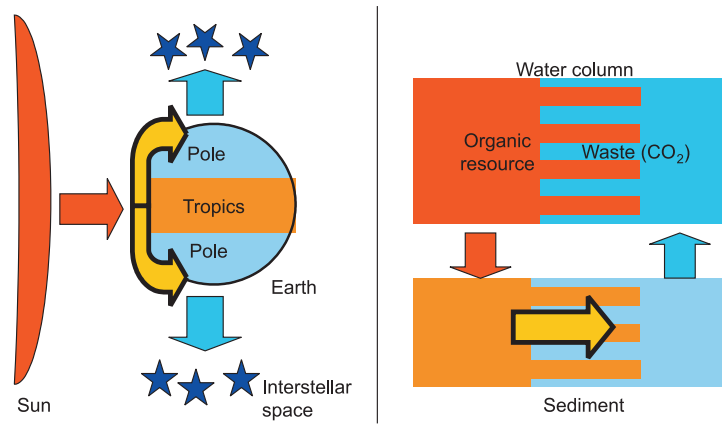


Figure 1.3: The correspondence between the sun-earth system and an oceanic sediment ecosystem.

Fig. 1.4 presents the common functioning. As the full description at this megascopic scale is too complicated, we will only describe the most basal functioning, by simplifying the model as a kind of 'black box' system (chapter 3). The model universe has an environment and a system, and both have two compartments, one for the resource and one for the waste. By using the energy or mass balance, the basic dynamics of the two system variables (corresponding with the two system compartments) can be written down as the input minus

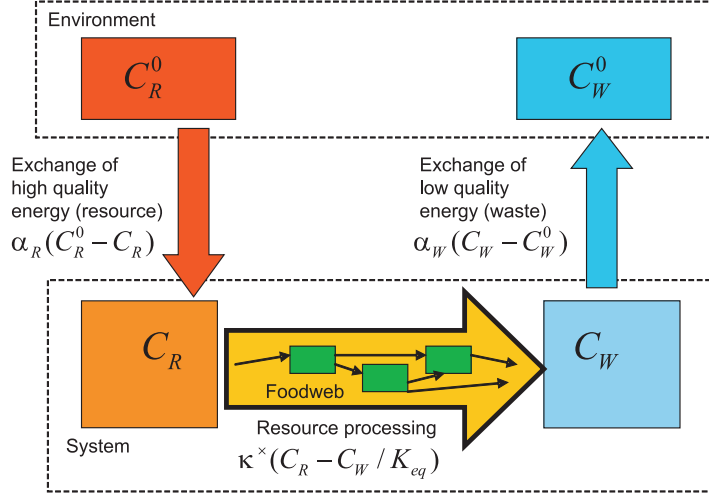


Figure 1.4: Common abstract structure of both systems of fig. 1.3.

the output of the respective compartments:

$$\frac{dC_R}{dt} = \alpha_R(C_R^0 - C_R) - \kappa^\times(C_R - C_W/K_{eq}), \quad (1.1)$$

$$\frac{dC_W}{dt} = \kappa^\times(C_R - C_W/K_{eq}) - \alpha_W(C_W - C_W^0). \quad (1.2)$$

For the ecosystem,  $C_R$  and  $C_W$  are the resource and waste concentrations. The superscript 0 refers to the environment, and these environmental quantities are constant.  $\alpha_R$  and  $\alpha_W$  are the constant exchange rate parameters and  $\kappa^\times$  is the specific resource processing rate. The superscript  $\times$  refers to the fact that it is an 'effective' rate: In general,  $\kappa$  might depend on hidden variables from the biota in the food web, but this ecosystem food web is supposed to be in a quasi steady state (constant concentrations of the biota), such that  $\kappa^\times$  can be treated as a function of the two remaining variables  $C_R$  and  $C_W$  only.  $K_{eq}$  is the equilibrium constant for the chemical resource-waste reaction.

The first result is that this quasi steady state dynamics can be translated to a basal climate dynamics in models studied by Paltridge, Kleidon, Lorenz, and many others [151, 98, 86]. (See table 11.2.) Write  $C_R$  as  $T_T$  (the average temperature at the tropics) and  $C_W/K_{eq}$  as  $T_P$  (the average temperature at the poles).  $\kappa^\times$  is now the atmospheric heat transport rate. As this factor depends on the complex atmospheric circulation processes, this 'effective parameter' is only well defined when the atmosphere is in a quasi steady state (the average distribution of eddy currents and fluid motions is constant).  $C_R^0$  and  $C_W^0/K_{eq}$  are now the temperatures that the tropics and the poles would attain in the absence of heat transport from the tropics to the poles (i.e. when  $\kappa^\times = 0$ ).

This rather trivial analogy might have a highly non-trivial implication. The above mentioned studies on climate systems of different planets resulted in the proposal of a 'maximum entropy production' (MaxEP) hypothesis (chapter 3 and section 5.5). The thermodynamic entropy production (EP) associated with

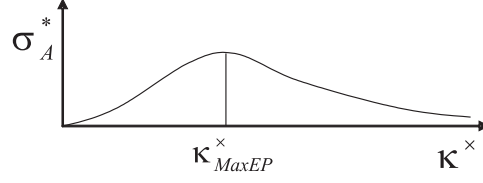


Figure 1.5: The maximum entropy production hypothesis: The atmospheric entropy production  $\sigma_A^*$  in function of the atmospheric heat transport coefficient  $\kappa^*$ .

the irreversible atmospheric heat transport is given by

$$\sigma_A^* = \kappa^* (T_T^* - T_P^*) \left( \frac{1}{T_P^*} - \frac{1}{T_T^*} \right). \quad (1.3)$$

The superscript  $*$  now denotes the complete steady state:  $T_T$  and  $T_P$  are also in their steady state values, and they are now functions of the three constant parameters  $\kappa^*$ ,  $\alpha_R$  and  $\alpha_W$ . Plotting  $\sigma_A^*$  against  $\kappa^*$  reveals that there is a value  $\kappa_{MaxEP}^*$  whereby the atmospheric EP is maximum (fig. 1.5). According to Paltridge, Lorenz et al., the experimentally observed  $\kappa^*$  lies close to  $\kappa_{MaxEP}^*$ , for different planetary systems.

We can ask the question: Is there a MaxEP principle associated with the ecosystem metabolism? Solving this, it first requires a reliable expression for the EP of the ecosystem metabolism. We have demonstrated that this EP (again in the steady state) can be written as

$$\sigma_{EM}^* = \kappa^* \left( C_R^* - \frac{C_W^*}{K_{eq}} \right) \ln \frac{K_{eq} C_R^*}{C_W^*}. \quad (1.4)$$

By looking at some real sediment ecosystems, [219] presented some first attempts to test whether  $\kappa^*$  lies close to the MaxEP value. For the moment (August 2007), the confirmations of the hypothesis are not yet convincing. Also theoretical explanations why this effective parameter should be close to its MaxEP value are still lacking. As the complete ecosystem food web or the turbulent atmospheric system are highly complex, one might hope that a more simple emergent behavior appears. The MaxEP hypothesis is such a candidate, and some people are inspired by the foundation of thermodynamics on statistical mechanics, to believe that, if the MaxEP hypothesis would turn into a real principle, a statistical law of large numbers might lie at its roots.

Let us now look at a less complex scale, a single laminar convective fluid motion or a simple food web (chapter 9). The most simple non-trivial food web one can think of is a resource-consumer system, with an additional variable, the consumer concentration  $C_C$ . The ecosystem metabolism factor can be written as the sum of an abiotic conversion parameter and a term linear in  $C_C$ :

$$\kappa_{EM} = \kappa_{AC} + g_{CR} C_C. \quad (1.5)$$

$g_{CR}$  is the growth rate of the consumer feeding on the resource. The dynamics of the consumer is given by the biomass growth minus the biomass decay:

$$\frac{dC_C}{dt} = q_{CR} g_{CR} C_C (C_R - C_W / K_{eq}) - d_C C_C. \quad (1.6)$$

This equation, together with (1.1), form a rather 'universal' dynamics, as our most intriguing result of our work shows that they can be translated into the simplified dynamical equations for Rayleigh-Bénard convective fluid cells (on the condition that we take the limit  $\alpha_W \rightarrow \infty$ , which results in a constant  $C_W \approx C_W^0$ ). These cells arise when a horizontal fluid layer is heated from below. (See table 11.3.) The resource is then related with the heat energy at high temperature, the waste with the low temperature heat energy, the consumer concentration with the kinetic energy of the fluid motion, the external applied concentration gradient  $C_R^0 - C_W^0/K_{eq}$  with the external applied temperature gradient, the ecosystem metabolism with the total heat transport, the abiotic conversion with the heat conduction, the biotic activity with the heat convection, the biological 'yield' factor  $q_{CR} \leq 1$  with a geometric factor (related with the size) of the convective fluid cells, the growth rate  $g_{CR}$  with the buoyancy force and the decay rate  $d_C$  with the fluid viscosity.

This strongly confirms the equivalence between the fluidal and the ecological systems. As a consequence of this correspondence between the dynamics, we can study what happens if different convection cells with different sizes compete with each other. When different biological consumers compete for the same resource, a well known law in ecology says that the consumer with highest evolutionary fitness, given by  $q_{CR}g_{CR}/d_C$ , survives and the other species go extinct. Translating this fitness to the fluid system, and maximizing it with respect to a geometric factor (width/height), gives the experimentally correct result that the width equals  $\sqrt{2}$  times the height.

One can speculate further on this idea (chapter 10). One can introduce more species, such as predators, in order to gradually build up more complex food webs. Can the concept of a food web be translated to fluid systems? Can hurricanes or even the whole earth atmosphere be represented by a food web, whereby different fluid motion patterns (eddy cells of different sizes) tap energy from each other, predate on each other or compete for heat and kinetic energy? Some indications (such as the similarity between turbulent cascades [9] and trophic cascades) affirm this new point of view.

The above results and new ideas all look very promising. Having derived a simple expression for the ecosystem EP, we are also able to answer some other interesting questions (chapter 6):

- If there are multiple steady states, does the most stable steady state have a higher EP than the other steady states? This question might be relevant for studying catastrophic regime shifts between multiple steady states, an important issue in theoretical ecology, see Scheffer et al. [176].
- Does the (total) EP increase when the system is driven further out of equilibrium (higher external gradient)? This question is related with the work by Kay and Schneider [179]. It might be relevant for the assessment of environmental changes (e.g. increased feeding) or the study of spatial differences in depositing rates in chemotrophic sediment ecosystems or irradiation in phototrophic ecosystems.
- Does a living ecosystem have a higher EP than a non-living system with the same boundary condition? I.e. are biotic processes more irreversible than abiotic? This question is related with the hypothesis studied by e.g.

Ulanowicz and Hannon [199], and with the idea that living organisms are dissipative structures [88] (chapter 8).

- Does the EP increase under the process of evolution?

All these questions can be answered in the negative (at least at the macroscopic level, not at the megascopic scale), by looking at specific ecosystem models and calculating for each model the total steady state EP (the sum of the ecosystem metabolism EP and the 'mixing' EP due to the exchanges of resource and waste)

$$\sigma_{tot}^* = \kappa^* \left( C_R^* - \frac{C_W^*}{K_{eq}} \right) \ln \frac{K_{eq} C_R^0}{C_W^0}. \quad (1.7)$$

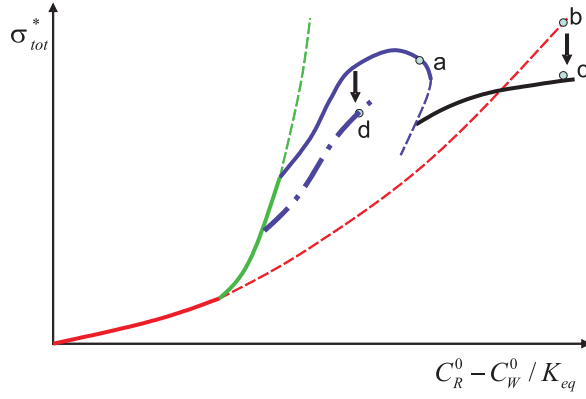


Figure 1.6: Qualitative figure of the total EP in a specific RCO ecosystem model. Solid lines are asymptotically stable states, dashed lines are unstable. The blue dotted-dashed line represents what happens after evolution (when a new omnivore outcompetes the old omnivore species): The blue solid line is shifted downwards.

Fig. 1.6 shows a qualitative picture of the  $\sigma_{tot}^*$ . The used model is an integration of different elements: a Lotka-Volterra resource-consumer-omnivore (RCO) dynamics (chapter 4) combined with a 'chemostat' dynamics with a biotic exchange limitation on the resource (chapter 8):

$$\begin{aligned} \frac{d}{dt} C_R &= (\alpha_R - l_C C_C - l_O C_O)(C_R^0 - C_R) \\ &\quad - (\kappa_{AC} + g_{CR} C_C + g_{OR} C_O)(C_R - C_W^0 / K_{eq}) \\ &\quad + d_C C_C + d_O C_O, \end{aligned} \quad (1.8)$$

$$\frac{d}{dt} C_C = q_{CR} g_{CR} (C_R - C_W^0 / K_{eq}) C_C - g_{OC} C_C C_O - d_C C_C, \quad (1.9)$$

$$\frac{d}{dt} C_O = q_{OC} g_{OC} C_C C_O + q_{OR} g_{OR} (C_R - C_W^0 / K_{eq}) C_O - d_O C_O, \quad (1.10)$$

with  $l_b$  the biotic exchange limitation parameters,  $g_{bb'}$  the growth rate parameters for  $b$  consuming  $b'$ ,  $q_{bb'} \leq 1$  the yields and  $d_b$  the biomass decay parameters. Choosing these parameters appropriately allows us to let the EP have the same qualitative behavior as in the figure.

In fig. 1.6, it is easy to see that there are unstable states (located on the dashed lines) with higher EP than corresponding stable states (for the same boundary condition, i.e. the same value of the external gradient  $C_R^0 - C_W^0/K_{eq}$ ). The system is driven further out of equilibrium when the external gradient increases. Therefore, the existence of a decreasing branch (around state 'a') means that the EP does not always increase. Next, the EP of the biotic state 'c' (containing a monoculture of the omnivore population) is lower than the abiotic, dead state 'b'. And if the evolutionary process (mutation and natural selection) would drive the growth rate  $g_{OC}$  of the omnivore preying on the consumer to higher values (i.e. the new omnivore with a higher growth rate outcompetes the old omnivore), then the EP might decrease, as can be seen from the downward shift of the blue branch to the dashed-dotted curve.

Note that the steady states of this model do not fit with the MaxEP hypothesis mentioned above. The studied ecosystem might be too simple, such that it will not correspond with a much more complex, turbulent fluid system. One can try to increase the complexity of the ecosystem model in order to see where MaxEP might become valid.

## Chapter 2

# Entropy production in ecosystems

### Abstract

Research in thermodynamic ecology is accompanied with some fundamental problems, related with the choice of variables and the expression for the entropy of biota and ecosystems. Our attempt is to study the entropy production (EP) for both chemotrophic and phototrophic ecosystems, and this requires an elaborate discussion on those problems. The ecosystems are modeled as a coupling between the system and the environment, which consists out of at least two reservoirs in internal equilibrium, but not in mutual equilibrium. This coupling drives the system out of thermodynamic equilibrium. By restricting the ecosystem to be in an entropic steady state, we can derive reliable expressions for the EP, even when the system is a black box, i.e. without specifying their internal structure and dynamics, or is not in local equilibrium, i.e. chemical potentials (of biota) are not well defined.

### 2.1 Introduction

For a long time, thermodynamic ecology only had its focus on the mass and energy balances in food webs. Recently, the physical description of ecosystems was enlarged by including the momentum balance [117]. But from a thermodynamic perspective, it is the entropy balance that is of particular importance, as the entropy balance allows us to derive the entropy production of ecosystems. As thermodynamic ecology studies energy transformation processes in ecosystems, these processes are irreversible and hence are accompanied with the production of entropy. The entropy balance was studied in e.g. [81]. However, these studies have a major flaw, as the major obstacle in thermodynamic ecology is that ecosystems can not be described as simple chemical reaction systems with chemical compounds in local equilibrium (see glossary for a definition), which means that e.g. chemical potentials are not well defined. This makes it highly difficult to speak of "the entropy" (or equivalently "the free energy" or "the chemical potential") of living organisms.

In this chapter and the next, we want to derive reliable expressions for the

entropy production (EP) for ecosystems<sup>1</sup>, not only because there is a need for a more rigorous study of the ecosystems entropy balance, but also because the EP is a rather elegant and fundamental property in irreversible thermodynamics. And above all, as we will see in later chapters, the EP is a potential candidate for an ecological goal function.

The first part of this chapter discusses the fundamental problems that we encounter in thermodynamical ecology. The rest of the chapter is divided in two sections, basically because there are two kinds of energy resources that are relevant for ecosystems: chemical compounds and photons. Both can carry energy that drives all the processes, and therefore, thermodynamic ecology makes the important distinction between chemotrophic and phototrophic ecosystems (see glossary for definitions). Both types of ecosystems will be studied in a 'black' box way: We do not look at the ecosystem functioning, but we only consider the exchanges between the ecosystem and its environment. In later chapters the black box ecosystems will be systematically colored up by studying concrete and well known ecosystem dynamics.

### What strategy to use?

Let us briefly summarize our choice of strategy that we will apply in this chapter and the next. There are two options in the study of the entropy balance for ecosystems. First, one can extend the classical formalism of non-equilibrium thermodynamics, the local equilibrium thermodynamics [88], to systems that are not in local equilibrium. This is very difficult as one has to extend classical thermodynamic notions, such as temperatures and chemical potentials, to a regime where they are not well defined anymore. Therefore, we will follow a second, much easier strategy. We will start with the classical formalism and derive an expression for the EP for local equilibrium. Next, we will find restrictions (such as steady state conditions) such that this EP expression becomes independent on the chemical potentials of specific chemical compounds. Finally, these specific chemical compounds are re-interpreted as organisms. As our EP now is independent on dubious quantities such as those 'biotic' chemical potentials, we are allowed to relax the local equilibrium condition (at the cost of requiring others, such as steady state conditions).

## 2.2 Fundamental problems in thermodynamic ecology

In our study of thermodynamic ecology, we encounter four basic problems.

### Choice of variables

*What are the proper variables to study a rabbit population? The number of rabbits? Or their sizes, colors, or the position of their left ears?*

The first step in modeling physical or ecological systems, is choosing a proper set of macroscopic variables. To study the temporal/spatial behavior of systems, we require that the variables obey an autonomous (closed) set of dynamical

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<sup>1</sup>Chapter 4 comments on 'unreliable' expressions for the EP that are studied in the literature.

equations, otherwise the dynamics can not be solved. We will write these *chosen macroscopic variables* as  $C_i(t)$ , with  $i$  indexing the different variables, and they obey the dynamics which is formally represented as

$$\frac{dC}{dt} = \sum_{\alpha} F_{\alpha}. \quad (2.1)$$

These equations are e.g. the energy, mass or momentum balances, when the variables represent resp. internal energies, particle numbers (local concentrations) or (fluid) velocities. The fluxes  $F_{\alpha}(C)$  are associated with transport (e.g. diffusion) or transformation (e.g. chemical reaction) processes. The dynamics is closed when these fluxes are functions of only the variables  $C$ .

The problem is not only that it might be difficult to find the proper variables that obey an autonomous set of dynamical equations, but above all that our chosen set of variables might not be sufficient for a thermodynamic description. Do the chosen variables uniquely determine the entropy of the system? If we have an entropy expression  $S(C_i, E_j)$ , it will be most likely a function of not only the chosen macroscopic variables  $C_i$ , but also of some 'extra' variables  $E_j$  that are not explicitly modeled. The 'chosen' and the 'extra' variables will all be called '*entropic variables*', i.e. these are the variables that completely specify the entropy.

To summarize, we can formulate the first problem in thermodynamic ecology as: *The set of entropic variables is typically larger than the set of chosen variables.* How are we going to deal with this problem? What variables are we going to choose? We want to stay as closely as possible connected to well known models in theoretical ecology. Therefore, our chosen variables will be so called '*ecological*' variables, i.e. variables that are studied in most ecological modeling. They typically consist out of the concentrations of bacteria or the biomasses of prey or predator species, denoted with  $C_B$ . These variables appear in Lotka-Volterra predator-prey systems, which will be studied in later chapters. However, we will see that from a thermodynamic perspective, it is important to include more variables, as the organisms do not grow on nothing. Organisms need an energy resource ( $C_R$ ) and this resource is degraded into waste products ( $C_W$ ). Furthermore, there might be other variables (temperatures, pressures, concentrations of other compounds,...). We will see soon how we will deal with these 'extra' variables.

### Ecosystem entropy and biotic chemical potentials

*What is the entropy or the chemical potential of a rabbit population? Is it different from a fox population of the same biomass?*

The entropy counts the number of microstates compatible with a macroscopic state, and the latter state is determined by the chosen set of macroscopic variables. As there is some arbitrariness in the choice of macroscopic variables, there is some arbitrariness in the entropy as well. But for systems in local thermodynamic equilibrium [47, 88], there exists an appropriate set of variables that specify the local entropy, the entropy of a local site of the system. These variables are the extensive quantities, such as internal energies  $U$ , volumes  $V$  and particle numbers  $N_i$  (with concentrations  $C_i = N_i/V$ ). We will not discuss the conditions for local equilibrium, but suffice it to say that the conjugate intensive

variables (resp. temperature  $T$ , pressure  $p$  and chemical potential  $\mu$ ) are well defined. They can be obtained by partial differentiation of the entropy. E.g. the chemical potential of particles of type  $B$  is

$$\mu_B = \frac{\partial S(U, V, N_i)}{\partial N_B}. \quad (2.2)$$

So what happens if we apply local equilibrium chemical thermodynamics to ecosystems? More specifically, if  $N_B$  now represent the number of organisms (or the biomass) of the species  $B$ , what is  $\mu_B$ , the biotic chemical potential? First, it might be a very complex function of the chosen ecological variables  $C_i$ . Second, it might not only be a function of the ecological variables, but also of the extra, hidden variables that are not modeled. Including these variables in the model might destroy the autonomy of the dynamical equations. But most importantly, the local equilibrium condition might not be valid for real ecosystems and real biota. Therefore,  $\mu_B$  might not even be well defined.

This is the second fundamental problem in thermodynamic ecology. The entropy production for chemical reaction systems depend on the chemical potentials of the involved chemical compounds. Therefore, if we would apply the chemical thermodynamics formalism to ecosystems, the EP of ecosystem processes will generally depend on the biotic chemical potentials of the involved organisms. How are we going to handle this problem? We have no ambition to try to calculate the entropy or the chemical potential of organisms and ecosystems (we will briefly come back on this major unsolved problem in chapter 7). But as we will see, there is a way to avoid this second difficulty: applying some assumptions and restrictions, our EP expression can be written in such a way that it no longer explicitly contains the biotic chemical potentials.

### System-environment distinction

*What is the environment of a rabbit population? The grass, the air, or the sun?* Why are ecosystems operating far from thermodynamic equilibrium? Because they are coupled with an environment that drives the system out of equilibrium. There is continuous exchange of matter or energy between system and environment. But here comes the third fundamental problem: How to characterize the distinction between ecosystem and environment? In a lot of studies in thermodynamic ecology (e.g. [81]), the environment is incorrectly modeled as one (big) compartment that exchanges matter and energy with the system. However, the environment itself is also not in equilibrium, otherwise it would not be able to drive the system out of equilibrium.

We will deal with this issue by a very simple modeling approach: We assume that the environment is in local equilibrium, and we divide it into *at least two* reservoirs instead of one global compartment. These reservoirs should be in *internal equilibrium*, but they are not in *mutual equilibrium*. Secondly, the reservoirs are very large, such that they have very long characteristic timescales. In other words, the intensive thermodynamic quantities (temperature, concentrations,...) of the environment are to a good approximation fixed. Finally, to drive the system out of equilibrium, one reservoir should have a high energetic quality (e.g. high chemical potential), and the other should have a low energetic quality (low chemical potential). As we will see later, the quality difference is a measure for the driving force. The first reservoir is called the resource reservoir

$R$ , the second contains the waste  $W$ . Environmental quantities  $C^0$  are constant, and therefore they are written with a superscript 0.

We will see that for our study of the EP, it is sufficient to assume that only the environment is in local equilibrium. The ecosystem is allowed to be outside local equilibrium. This relaxes the local equilibrium formalism to a *quasi local equilibrium*, whereby only the environment (and perhaps a few compartments of the ecosystem) need to be in local equilibrium. As real ecosystem organisms or food webs are most likely not in local equilibrium, the quasi local equilibrium property is more than welcome.

### Equilibrium and (quasi) steady states

*If the rabbit population stays constant, is it in equilibrium or a steady state? Is the entropy of such a constant population also constant or does it make a difference whether the rabbits were running around or standing still?*

The most general states are transient states, whereby variables might change in time. When some variables are constant, the system is in a (quasi) steady state, and the constant values are written as  $C^\times$ . When all ecological variables are constant, the system is in a ecological steady state<sup>2</sup>. The ecological variables are now written as  $C^*$ , and the fluxes are related as  $\sum_\alpha F_\alpha = 0$ . When every independent flux  $F_\alpha = 0$ , the ecological variables are in thermodynamic equilibrium, denoted with  $C^{eq}$ .

However, the above discussion about 'chosen' and 'extra' variables needs some further comments. Entropic steady states are states whereby all entropic variables of the ecosystem are constant. Entropic quasi steady states are a small generalization of such steady states: Only the 'dangerous' entropic variables are constant. These variables are the extra variables  $E_i$ , together with all other chosen variables that represent quantities that are not in local equilibrium. For example, the biomass  $C_B$  is definitely a 'dangerous' entropic variable, as its corresponding chemical potential might not be well defined. But the concentration of e.g. the waste product  $CO_2$  is not 'dangerous' when its chemical potential  $\mu_W$  is well defined.

The notion of entropic steady states is important due to the following: As we will see in the next chapter, we will derive an EP expression, and by restricting the system to be in an *entropic (quasi) steady state*, the terms containing the biotic chemical potentials drop out of the expression. Therefore, our fundamental assumption to avoid the above mentioned central difficulty is that the system operates in the entropic (quasi) steady state.

It is important to stress that the condition for entropic steady states is not that self-evident. The notion of a steady state is highly dependent on the chosen variables. As an example, consider a water flow. If the variables are the positions of the fluid, then the steady state is a static state, with zero flow. But if the velocities are the variables, the steady state is given by a stationary flow. And if the accelerations are the variables, then the steady state is a uniform accelerated flow, etc. It is clear that in living ecosystems, there are always changes, transformations, flows,...

So we encounter our next problem: How do we know that a system is in an entropic steady state? Again, we clash with the problem of the choice of ecosy-

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<sup>2</sup>Steady states are sometimes also called 'ecological equilibrium', but we will not use this language as it might be confusing with 'thermodynamic equilibrium'

stem variables. Typical models in theoretical ecology only have the biomasses (concentrations) of the biota as ecological variables. Steady states for these variables can be studied, but these ecological steady states are *not* necessary entropic steady states, because the entropy might depend on other variables which were not taken up in the set of dynamical equations. These 'entropic but not ecological' variables might be 'invisible' for the ecological modeler, but if they have sufficiently short relaxation times, one can take them to be in a constant steady state value. Hence, if this 'short relaxation time' assumption is valid, we can take all 'invisible' variables to be constant. Therefore, if also all the 'visible', ecological variables are in a steady state, then all entropic variables are constant, and therefore the ecosystem entropy is constant. As we will see, this constancy means that the derived EP expressions contain no contributions from changing ecosystem variables, only the environmental extensive variables are changing. And this is the basic reason why we can still study the EP even though we have no knowledge of ecosystem entropies or biotic chemical potentials. The system can be considered as a 'black box' and can even be outside local equilibrium. We only have to assume that entropic (quasi) steady states are to a good approximation equivalent with ecological (quasi) steady states, so that is what we will do from now on.

But one problem remains: Real ecosystems often do not settle in steady states. What about oscillatory, quasi periodic or chaotic states? Perhaps one can take suitable time averages of those attractor states (see glossary). And what about fluctuations, perturbations, evolution,...? All these questions are relevant, but we will not deal with them in this work. We will only study deterministic equations with steady state solutions.

## 2.3 Chemotrophic ecosystems

In this section we will set up the basics for a thermodynamic description of chemotrophic ecosystem. First we will describe a chemostat ecosystem, the primordial example of a laboratory set-up that we will model in later sections. Next, we present a schematic overview of approximations and assumptions in order to obtain a range of possible EP expressions, some more reliable than others. In this chapter we will look at the system as a 'black box'. In chapter 3, this system will be refined further (a 'grey box') and chapter 4 presents a concrete set of ecosystems (a 'colored box'), with a specific dynamics.

### 2.3.1 The chemostat

Figure 2.1 shows the chemostat system, which is a Continuous Stirred-Tank Reactor (CSTR) that contains different abiotic compounds as well as biotic species, and that is coupled with reservoirs with a continuous in- and outflow of chemical 'resource' and 'waste' compounds. These substances can chemically react inside the tank reactor. The chemical potential  $\mu_R^0$  of this environmental resource reservoir should be well defined and measurable. Therefore, the resource should be a rather simple chemical substrate. Prime examples are a solution of glucose ( $CH_2O$ ) for chemoheterotrophic ecosystems (see glossary), and methane ( $CH_4$ ) or hydrogen sulfide ( $H_2S$ ) for chemo-autotrophic systems. The resource exchange is performed by passive diffusion or active transport (pum-

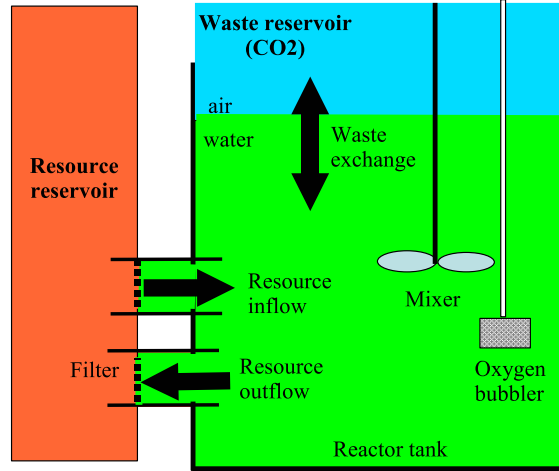


Figure 2.1: The chemostat (CSTR) system.

ping). In typical chemostat experiments, there is a wash out of organisms. But when organism that are not in local equilibrium enter a reservoir, the internal equilibrium property of the environmental reservoir is violated. Therefore, in our description it is necessary to place a filter at the exchange valves, so the organisms can not escape to the reservoir<sup>3</sup>.

The resource is degraded (e.g. oxidated) inside the reactor tank, to produce waste products. Prime examples for waste are  $CO_2$  for chemoheterotrophic and  $SO_4$  for chemo-autotrophic systems. The waste reservoir is e.g. the atmosphere or another aquatic reservoir, and again the exchange is passive diffusion or active transport. The chemical potential  $\mu_W^0$  of the waste reservoir should be well defined and measurable.

The temperature and pressure are assumed to be homogeneous, constant and equal in both system and environment. The fluid inside the reactor tank is mixed to a homogeneous solution. In this way, we only have to model global variables obeying ordinary differential equations, avoiding the more difficult study of partial differential equations. The oxygen concentration in the ecosystem is an extra variable that we will not model. As the ecosystem entropy might depend on it, we have to keep it constant in the entropic steady state. An oxygen bubbler controls the oxygen concentration to a fixed value such that e.g. the oxidation rate does not depend on a variable oxygen concentration.

In this work, we will especially focus on chemoheterotrophic systems, as in these systems the organic chemical resource (e.g. glucose) serves two functions: energy resource and carbon nutrient (building block) for biomass production.

<sup>3</sup>As the organisms are not transported out of the system, we do not study classical chemostats [185]: In classical chemostat modeling, there is no biomass decay, but biomass wash out. In this work, we only study filter chemostats instead of classical chemostats. Although the mathematical formulation is roughly the same for both systems with and without filters, the thermodynamics is highly different. In particular, the thermodynamic description of classical chemostats encounter some serious problems.

### 2.3.2 Schematic derivation for the entropy production

We now present a schematic line of simplifications (fig. 2.2) that results in an array of possible EP expressions that we will use in later chapters. This pallet of strategies has two extremal end-member situations. One extremum focuses at the total EP in an entropic steady state. This gives the most reliable expression, which is applicable even when the ecosystem is not in local equilibrium. Knowledge of the thermodynamics of the biota in the ecosystem is not required. But on the other hand, it is not applicable to individual EP's for individual processes, nor is it applicable to the transient states. However, it is nonetheless an interesting quantity, with sufficiently rich behavior. Therefore, it will be used in most parts of our work. The other extremum has the advantages that individual EP's in the transients can be studied, but it is theoretically much more on shaky grounds, as it is only applicable when the thermodynamics of the ecosystem (variables, chemical potentials of biota, fluxes,...) is sufficiently known. In order for this approach to be valid, the system has to be in local equilibrium. As mentioned, this might not be valid for real ecosystems, but yet it remains an open question whether it is possible to find a correct level of description with suitable variables for ecosystems such that local equilibrium is valid, at least to a good approximation. Anyway, if a local equilibrium description turns out to be possible, for modeling simplicity, some assumptions on the chemical potentials and the dynamics of the biota are needed, but they might yet be highly unrealistic. Therefore, this approach will be used in only one part of this thesis, namely in chapter 7.

Let us now give in a more systematic way all the simplifications. The model universe is described by the total system which is energetically and materially isolated and has constant volume. The model universe should be in global equilibrium for the pressure and temperature. Next, this model universe should be divided into the ecosystem (at constant volume) and the reservoirs of the environment. The ecosystem is described by ecological variables that obey an autonomous set of dynamical equations. Each reservoir should be in internal equilibrium, having a constant and homogeneous concentration of one basic abiotic chemical compound. These chemical components can be classified as 'resource(s)' or 'waste(s)', depending on the energetic quality. Hence, we have:

- One (or more) homogeneous resource reservoir(s) of the environment. The chemical potentials of these environmental reservoirs should be well defined and measurable.
- A number of compartments for the ecosystem food web. The chemical potentials are not necessarily known.
- One (or more) homogeneous waste reservoir(s) of the environment. The chemical potentials should be known.

Next, the pallet of possible strategies appears. One end-member situation needs two final restrictions:

*Total EP:* First of all, we will not study the EP of singular processes, but we will only study the total EP of the total model universe.

*Entropic steady state:* Secondly, we will only look at the total 'entropic' steady states, i.e. the ecosystem entropy should be time-independent because all determinant entropic variables are in a steady state. We will assume that ecological steady states are entropic steady states.

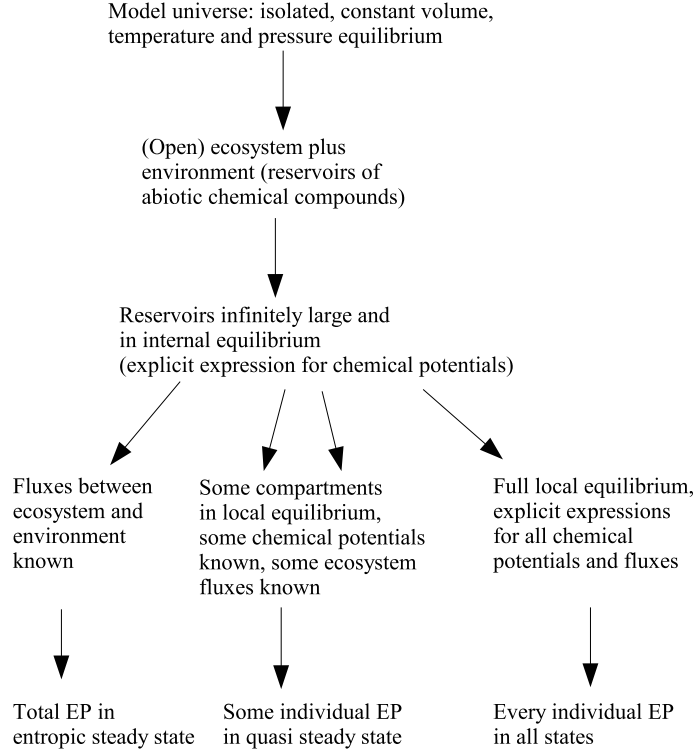


Figure 2.2: The simplifications in the derivation of EP expressions. The total EP  $\sigma_{tot}^*$  in the entropic steady state will be used in most parts of this thesis. The individual EP  $\sigma_{EM}^*$  for the ecosystem metabolism in a quasi steady state will be discussed in chapter 3. The individual EP's for all processes in all states will be dealt with in chapter 7.

As we will demonstrate in more detail in the next chapter, the obtained total steady state EP (when there is only one resource and one waste reservoir) looks like

$$T\sigma_{tot}^* = (\mu_R^0 - \mu_W^0) F_R^* = TX^0 F_R^*, \quad (2.3)$$

with  $X^0$  the external driving force and  $F_R^*$  the resource exchange rate, which in the steady state equals the total flux from the resource to the waste reservoir. The remarkable property is that we do not need to know the system variables, chemical potentials,... Whether the ecosystem is in local equilibrium or not, whether it is homogeneous or heterogeneous, simple or complex, contains sharks or dolphins, only the environment (the chemical potentials and the exchange flux) is important for this EP. The importance of the environment places also a new focus: Ecologists often focus on the ecosystem and its internal structure and functioning, neglecting the environment. But from a thermodynamic point of view it is precisely the latter that becomes important.

One can now gradually introduce new approximations, or take a more refined description. As an example, in chapter 3, a little extension is made. This allows to study the so called metabolic EP in a quasi steady state. By taking more and

more explicit expressions for the chemical potentials of the ecosystem compartments (such as the living organisms), and more and more explicit expressions for the fluxes (in function of the ecosystem variables) within the ecosystem, one can progressively study individual EP's. These EP's are now no longer required to be applicable for the entropic steady states only. The restriction that the system is in the entropic steady states can be gradually relaxed to the quasi steady and eventually the full transient states. Full knowledge of every flux and thermodynamic quantity allows us to look at EP for every process (e.g. biomass decay) and in each (transient or steady) state. In chapter 7, an example of this end-member scenario is given. The disadvantage of this strategy is that the theoretical expressions we will use might be highly unrealistic for real ecosystems (e.g. taking aquatic organisms as perfect and ideal solutes is far-fetched).

## 2.4 Phototrophic ecosystems

In most parts of this work, we will look at chemotrophic ecosystems. However, most ecosystems on planet earth are phototrophic, as photosynthetic organisms receive radiation energy from the sun. To give a flavor how to calculate the EP for phototrophic systems, we will briefly study the most simple type of such systems: planetary systems, such as the earth or Gaia (daisyworld) models [203]. These models describe systems (planets) that are materially closed but energetically open to the environment, which basically consists of the sun and the interstellar space. In this section we will only focus on the energy and entropy balances for such radiation systems, whereby the thorough discussions by Planck [156] on the thermodynamics of heat radiation will be useful. In chapter 8 we will explicitly introduce the biota by modeling the fractional area of the planet that is covered with biota. This fractional area will be a central variable, as it determines the EP of the planet.

### 2.4.1 The homogeneous planet

Consider a star (the sun) that radiates heat energy at constant high temperature  $T_H^0$  (e.g.  $\sim 5700K$  for the solar surface) towards a planet (the earth) at homogeneous but variable temperature  $T_E$  ( $\sim 300K$ ). The interstellar background has negligible temperature  $T_L^0 \approx 0$ . Sun and background are the environmental heat reservoirs.

#### The energy balance

Let us first study the energy balance for the earth. Our fundamental assumption is that both sun and planet have black body emission spectra, which means that the heat flux is proportional to  $T^4$ .

$$C_{V,E} \frac{dT_E}{dt} = F_H - F_E = \alpha_H (T_H^0)^4 - \epsilon_L T_E^4. \quad (2.4)$$

The first term is irradiation flux from the source<sup>4</sup>. The absorption factor  $\alpha_H$  expresses the fact that a part of the high frequency radiation is reflected, wit-

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<sup>4</sup>For the sun earth system, it is easy to demonstrate that  $\alpha_H = (1 - a_E) \frac{cr A_S A_E^{in}}{4 A_{SE}}$ , with  $a_E \leq 1$  the earth albedo,  $A_S = 4\pi r_S^2$  the area of the solar surface ( $r_S$  is the solar radius)

hout being absorbed by the system. There are two interesting types of models whereby the absorptivity depends on the system variables. The first type is studied in e.g. climatic thermostat models [53], whereby the albedo depends on the temperature of the system. The second type of models are famously known as Gaia models [203], whereby the albedo also depends on the biota (e.g. the area covered by biota). We will use a latter type of model in chapter 8. The second term in the energy balance is the earth emission flux<sup>5</sup>.

### The entropy balance

Roughly speaking, the absorption of a few high frequency photons and the emission of many low frequency photons increases the number of degrees of freedom and hence increases the entropy. The higher the absorption or emission, the higher the EP. How to calculate this EP?

The thermal heat radiation fluxes in the energy balance were all simplified to grey (emissivity  $e_E < 1$ ) or black ( $e_E = 1$ ) body spectra. In order to derive simple yet reliable expression for the EP, we assume that the planet is a black body emitter. Black body radiation obeys the relation  $S = (4/3)U/T$ , with  $S$  the entropy and  $U$  the internal heat energy. Consider a quantity  $dU$  that is emitted by the sun in time  $dt$ . It is easy to see that the entropy flux is

$$\frac{d_e S_S}{dt} = -\frac{4}{3} \frac{F_H}{T_H^0}, \quad (2.5)$$

with  $d_e$  the formal notation of the entropy emitted, and  $F_H = dU/dt$  the energy flux. But associated with this emission, there is an internal entropy production<sup>6</sup>

$$\frac{d_i S_S}{dt} = \frac{1}{3} \frac{F_H}{T_H^0}, \quad (2.6)$$

so the total entropy change inside the sun equals

$$\frac{dS_S}{dt} = -\frac{F_H}{T_H^0}. \quad (2.7)$$

Next, this package of energy is absorbed by the earth, and its entropy increases with  $dS_E = F/T_E$ . The total EP due to sun emission and earth absorption is therefore

$$\sigma_1 = \frac{d(S_S + S_E)}{dt} = \left( \frac{1}{T_E} - \frac{1}{T_H^0} \right) F. \quad (2.8)$$

This is the expression used by e.g. Kleidon [85] to study the EP of the earth. However, the earth also emits radiation with flux  $F_E$ , and due to this emission,

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and the factor  $1/4$  comes from a solid angle integration over the hemisphere [156].  $r = 8\pi^5 k_B^4 / 15h^3 c^3$  is the radiation constant.  $A_E^{in} = \pi r_E^2$  is the effective area (i.e. the cross section) of the incoming radiation at the earth ( $r_E$  is the earth radius), and  $A_{SE} = 4\pi r_{SE}^2$  is the area of the spherical shell with radius  $r_{SE}$ .

<sup>5</sup>For the sun earth system,  $\epsilon_L = e_E \frac{c r_A E}{4}$ , with  $e_E \leq 1$  is the ecosystem emissivity and  $A_E$  the earths surface.

<sup>6</sup>The factor  $1/3$  comes from the pressure relation  $p = 1/3u$ , [156].

there is internal EP  $d_i S_E = (1/3)F_E/T_E$ . When the earth is in a steady state, we have  $F_H^* = F_E^*$ , and therefore

$$\sigma_2^* = \frac{1}{3} \frac{F_H^*}{T_H^0} + \frac{4}{3} \left( \frac{1}{T_E^*} - \frac{1}{T_H^0} \right) F_H. \quad (2.9)$$

The first term is the sun emission EP and this is not relevant for climate and ecosystem modeling. Therefore, the second term is used by e.g. Essex [58] as the earth EP. It is 4/3 times  $\sigma_1$ , and therefore, it suffices to study only (2.8). The EP of the spreading and dilution of the emitted radiation of the earth into the background is also not relevant.

Equation (2.8) is our basic expression for the EP of phototrophic ecosystems, such as the living earth. It is valid in the entropic steady state. One can also try to generalize the description, and a scheme similar to fig. 2.2 might be possible. These generalizations allow us to study transient states, but we will not consider them in this work.

Let us summarize the most important assumptions and restrictions for phototrophic ecosystems. The phototrophic model universe is isolated at constant volume. This model universe is divided in a materially closed ecosystem and the environment. The ecosystem has ecological variables that obey a set of autonomous dynamical equations. The environment consists of one or more radiating black bodies at constant internal temperatures. The ecosystem emission spectrum is black (i.e. the emissivity is unity), the ecosystem temperature  $T_E$  is homogeneous, the albedo is independent of the irradiation frequency and the temperatures, but it might depend on the ecosystem variables, and the ecosystem is in an ecological (=entropic) steady state.

## Chapter 3

# A thermodynamic perspective on food webs: quantifying the entropy production associated with resource processing

### Abstract<sup>1</sup>

Because ecosystems fit so nicely the framework of a 'dissipative system', a better integration of thermodynamic and ecological perspectives could advance the quantitative analysis of ecosystems. One obstacle is that traditional food web models are solely based upon the principles of mass and energy conservation, while the theory of non-equilibrium thermodynamics principally focuses on the concept of entropy. To properly cast classical food web models within a thermodynamic framework, one requires a proper quantification of the entropy production that accompanies resource processing of the food web. Here we present such a procedure, which emphasizes a rigorous definition of thermodynamic concepts (e.g. thermodynamic gradient, disequilibrium distance, entropy production, physical environment) and their correct translation into ecological terms. Our analysis provides a generic way to assess the thermodynamic operation of a food web: all information on resource processing is condensed into a single resource processing constant. By varying this constant, one can investigate the range of possible food web behavior within a given fixed physical environment. To illustrate the concepts and methods, we apply our analysis to a very simple example ecosystem: the chemotrophic chemostat. Finally, we put forward a maximum entropy production hypothesis and make the connection with the global climate system.

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<sup>1</sup>This chapter is a shortened and modified version of [219].

### 3.1 Introduction

Up to now, the marriage between ecology and thermodynamics has been a rather difficult one. Although the need for a thermodynamic perspective on biological processes has long been recognized [182], these two disciplines have shown little integration over the past 50 years. For example, the term 'entropy', which is a key thermodynamic concept central to the Second Law of thermodynamics, does usually not feature in standard ecological textbooks, e.g. [114, 13, 30]. The application of non-equilibrium thermodynamics in biology is classically restricted to the subcellular level, where metabolic processes are cast within the formalism of chemical thermodynamics [171, 90]. Yet, when moving to the community or ecosystem level, these concepts and methods are no longer invoked.

This is surprising, as ecosystems particularly fit what thermodynamicists call 'open dissipative systems', as investigated by Ilya Prigogine and co-workers some decades ago [65, 134]. Such dissipative systems experience a continuous through-flow of mass and/or energy, which is 'degraded' from a high-quality to a low-quality form. In thermodynamic terms, this 'quality degradation' is termed dissipation, and the physical quantity that quantifies dissipation is the entropy production. The archetypical illustration of dissipation in ecology is found when looking at the biosphere in a black-box fashion [199]. The earth as a whole thrives on an input of high-quality solar radiation, and releases roughly the same amount of energy back to the space as low-quality heat radiation. The quality difference between incoming short-wavelength and outgoing long-wavelength radiation is exploited by photosynthetic organisms (phytoplankton, trees, grasslands) that build up the organic resources that sustain other trophic levels.

The dichotomy between ecology and thermodynamics is nicely illustrated by the distinct 'model currencies' that are in use within different research communities. In the field of ecological modeling, the default variables are mass and energy, of which the associated conservation equations form the central heart of food web and ecosystem models [93, 114, 67, 96]. The theory of non-equilibrium thermodynamics basically extends this mass/energy toolbox with the concept of entropy, and the principal focus in thermodynamic analysis is the proper quantification of entropy production within the various model systems [134, 88]. Yet, until now, these two ways of describing natural systems are poorly cross-linked. The concept of entropy remains highly enigmatic to most ecological modellers, while thermodynamicists have not applied their entropy production calculations to actual ecosystems.

In recent years, there's a growing number of publications that specifically aim to close the gap between ecology and thermodynamics (see reviews in [79, 81, 181]). Given its emphasis in non-equilibrium thermodynamics, one would expect the entropy concept to play a dominant role in this emerging field of 'thermodynamic ecology'. Surprisingly however, this is not the case. The prevalent idea is that the standard mass/energy/entropy toolbox of classical non-equilibrium thermodynamics is not suitable for the description of ecological processes [79, 81]. In this view, ecology is of inherently different nature than the dissipative phenomena usually dealt within 'abiotic' non-equilibrium thermodynamics, so that additional constructs and new rules must be introduced to fully describe an ecosystem's functioning. As a result, a number of novel 'ecological' concepts have been forwarded as essential complements to the standard entropy

concept, including energy [141], exergy [179], eco-exergy [189] and ascendancy [198]. However, the use of these newly defined properties does not come without problems. The first problem is the loose and verbal use of thermodynamic language, and the highly qualitative way in which these concepts are used. Secondly, each of these concepts has its proponents, but the exact interrelation between them remains unclear. Thirdly, and more fundamentally, the question remains whether the standard mass/energy/entropy toolbox of non-equilibrium thermodynamics is really insufficient to analyze ecosystem functioning.

In our view, the standard formulation of non-equilibrium thermodynamics has not been explored to its full potential within an ecological context. Here, the goal is to examine how this theory can be applied in a strict 'orthodox' fashion to the analysis of resource processing within ecosystems. In other words, we will not invoke any 'ecological' additions or modifications of the conventional theory [65, 88]. As noted above, entropy is the central variable in the analysis of dissipative systems, and hence, our prime concern will be to develop a consistent procedure to calculate the entropy production within an ecosystem. To this end, we need to correctly translate thermodynamic concepts (e.g. dissipation, thermodynamic gradient, distance from equilibrium, entropy production) into an ecological context. To illustrate the concepts and methods, we apply our analysis to a very simple example ecosystem: a chemotrophic food web in a chemical reactor tank. This will show how classical food web models can be cast within the standard framework of non-equilibrium thermodynamics.

## 3.2 Model formulation

### 3.2.1 Resource processing in a chemostat ecosystem

The model analyzed here forms an idealization of a chemo-heterotrophic chemostat ecosystem [185] - see Fig. 2.1. The ecosystem is fueled by an input of organic matter (e.g. glucose), which is given the simple stoichiometry  $\text{CH}_2\text{O}|_{\text{R}}$ . Some of this resource is taken up by the food web and converted into biomass, represented by the reaction



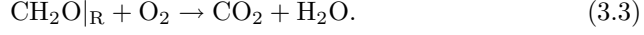
with the associated rate  $F_{BS}$  (Biomass Synthesis). A crucial aspect of our model is that the food web is considered a true black box, and no a priori assumptions are adopted about its internal structure. Accordingly, the simplified stoichiometry  $\text{CH}_2\text{O}|_{\text{B}}$  generically represents the biomass stored in all trophic compartments. Furthermore, we assume that biomass is simply assembled from elementary building blocks of resource. More elaborate descriptions of stoichiometry are possible [188], but these rapidly increase model complexity. The simplicity of reaction (3.1) helps us to emphasize those features of food webs that are important from a thermodynamic perspective.

The turn-over (decay) of biomass is described by the opposite transformation



with associated rate  $F_{BR}$  (Biomass Recycling). Biomass turn-over thus means that biomass simply disassembles into basic building blocks, which become again

available for biomass synthesis or respiration<sup>2</sup>. Accordingly, the net production by the food web becomes  $F_{NP} = F_{BS} - F_{BR}$ . Finally, the decomposition (oxidation) of organic matter is described by the simplified transformation

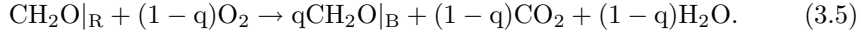


Here,  $\text{O}_2$  represents the electron acceptor that is used, while  $\text{CO}_2$  and  $\text{H}_2\text{O}$  stand for the various end-products that result from organic matter decomposition. Effectively, reaction (3.3) symbolizes the core dissipative process within our ecosystem: high-quality resources ( $\text{CH}_2\text{O}$ ,  $\text{O}_2$ ) are converted into low-grade waste products ( $\text{CO}_2$ ,  $\text{H}_2\text{O}$ ). The associated reaction rate is referred to as the 'ecosystem metabolism', denoted  $F_{EM}$ . We consider two distinct pathways of organic matter decomposition, termed 'abiotic conversion' (rate  $F_{AC}$ ) and 'biotic conversion' (rate  $F_{BC}$ ), so that

$$F_{EM} = F_{AC} + F_{BC}. \quad (3.4)$$

The abiotic pathway  $F_{AC}$  represents a purely chemical oxidation mechanism (i.e. not biologically catalyzed), which is a slow process that is always present in the background. The biotic pathway  $F_{BC}$  results from the metabolism of the food web, and thus represents the overall respiration of the food web. Under natural conditions, the biotic conversion of organic matter will exceed by far the purely chemical decomposition. Effectively, the flux  $F_{AC}$  would only be important when the chemostat is treated by a biocide killing off all biological activity. Still from a theoretical viewpoint, it is useful to explicitly account for the abiotic pathway (as shown below).

The reactions (3.1)-(3.3) cannot occur independently however. The synthesis of biomass (3.1) does not occur spontaneously, and must always be coupled to respiration (3.3). This coupling between anabolism and catabolism can be formally represented as



The yield factor  $q$  is always smaller than one, as it represents the consumer biomass that results from the assimilation of one unit of resource. Or equally,  $1 - q$  denote the respiration costs associated with biomass synthesis (activity respiration). In general,  $q$  cannot be regarded as a constant, but will depend on the structure of the food web. The rate of reaction (3.5) is termed the resource uptake  $F_{RU}$ , and the relations  $F_{BC} = (1 - q)F_{RU}$  and  $F_{BS} = qF_{RU}$  hold. Eq. (3.5) shows that in the chemo-heterotrophic ecosystem, the resource plays a dual role, one as an energy carrier and one as a building block.

### 3.2.2 Simplified ecosystem model

The mass flow diagram of Fig. 3.1 gives the general description which strips the ecosystem down to its barest essentials. In our model analysis, we will principally track the behavior of two components, termed resource (R) and waste (W), which are respectively identified as  $\text{CH}_2\text{O}|_R$  and  $\text{CO}_2$ . Although we will formally write a mass balance for the biomass  $\text{CH}_2\text{O}|_B$ , our black box analysis

<sup>2</sup>In later chapters we will include an additional decay process, basal maintenance, described by the transformation  $\text{CH}_2\text{O}|_B + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O}$ .

will not explicitly consider the resulting biomass dynamics, nor its partitioning over the trophic compartments. By principally focusing on the dynamics of  $\text{CH}_2\text{O}|_R$  and  $\text{CO}_2$ , we arrive at a description that is simple and mathematically manageable, while retaining the essential aspects of the problem.

Our model incorporates three basic assumptions.

- (1) No substrates other than the resource  $\text{CH}_2\text{O}|_R$  are limiting (other substrates are sufficiently abundant such that biological processes are only dependent on the resource concentration).
- (2) The exchange of electron acceptor with the environment is considered sufficiently fast, so that the concentration of  $\text{O}_2$  remains at a steady, non-limiting level (justifiable when an oxygen bubbler is placed in the chemostat). As a result, we do not need to include a mass balance for the electron acceptor  $\text{O}_2$ , nor do we provide one for  $\text{H}_2\text{O}$ .
- (3) Temperature effects can be ignored, and so both ecosystem and external environment remain at the same constant temperature  $T$  (this is again a suitable assumption for laboratory chemostat ecosystems).

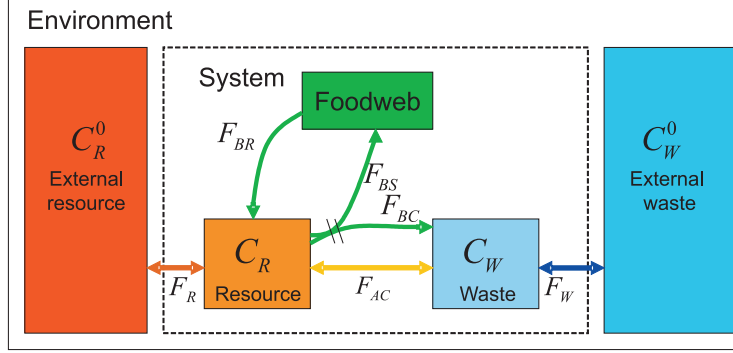


Figure 3.1: Idealized flow scheme of the chemo-heterotrophic ecosystem. Six interactions occur between five reservoirs. The cross bars indicate that the flows  $F_{BS}$  and  $F_{BC}$  are coupled.

The scheme in Fig. 3.1 represents our 'model universe', and incorporates two parts, termed 'ecosystem' and 'environment'. Both ecosystem and environment contain one resource (R) and one waste (W) compartment, while the ecosystem additionally contains the biomass compartment (B) of the food web. The principal difference between the internal and the external compartments is their size. The compartments in the environment are considered 'infinite' reservoirs, so that the concentrations  $C_R^0$  and  $C_W^0$  are fixed model parameters. In contrast, the internal ecosystem compartments have a finite size, and the concentrations  $C_R$ ,  $C_W$  and  $C_B$  are state variables that need to be determined by some suitable mass balance equations (see below). The net exchange of resource and waste between ecosystem and environment is represented by the flows  $F_R$  and  $F_W$ . This way, our model includes five independent flows in total:  $F_R$ ,  $F_W$ ,  $F_{AC}$ ,  $F_{BC}$  (coupled with  $F_{BS}$ ) and  $F_{BR}$ .

### 3.2.3 Mass balance formulation

The variables within the ecosystem are subject to the mass conservation equations

$$\frac{dC_R}{dt} = F_R - F_{AC} - F_{BC} - F_{BS} + F_{BR}, \quad (3.6)$$

$$\frac{dC_W}{dt} = -F_W + F_{AC} + F_{BC}, \quad (3.7)$$

$$\frac{dC_B}{dt} = F_{BS} - F_{BR}. \quad (3.8)$$

where the fluxes  $F_\alpha$  are expressed as mass per unit of volume and time. These mass balances include six fluxes that need suitable constitutive expressions. Three fluxes ( $F_R$ ,  $F_W$ , and  $F_{AC}$ ) are governed by strictly abiotic processes, and can be directly parameterized. The abiotic conversion of resource is modeled by the standard kinetic rate expression

$$F_{AC} = \kappa_{AC} \left( C_R - \frac{C_W}{K_{eq}} \right). \quad (3.9)$$

which assumes that the reaction rate is linear in the concentrations. The constant rate parameter  $\kappa_{AC}$  (units of inverse time) specifies the time scale over which the incoming resource is degraded in the absence of biota. The quantity  $K_{eq}$  denotes the thermodynamic equilibrium constant of the chemical reaction (3.3). It is a fixed physical constant that is not influenced by the biology, and which attains a specific value at a given temperature.

The exchange  $F_R$  and  $F_W$  between the internal ecosystem compartments and the external surroundings are determined by the physical transport coefficients  $\alpha_R$  and  $\alpha_W$  (units of inverse time). The resulting constitutive relations are

$$F_R = \alpha_R (C_R^0 - C_R), \quad (3.10)$$

$$F_W = \alpha_W (C_W - C_W^0), \quad (3.11)$$

This linearized transfer is the standard way of modeling the exchange with the environment in ecological models [194, 96].

Given the above explicit expressions for the abiotic fluxes  $F_R$ ,  $F_W$ , and  $F_{AC}$ , only the biotic fluxes  $F_{BS}$ ,  $F_{BR}$  and  $F_{BC}$  need further specification. The constitutive expression for these biotic fluxes will depend on the food web that mediates these fluxes, and so the structure of this food web needs to be first specified. However, even without explicitly describing the food web, it is possible to analyze the effect of the food web on resource processing (as shown below).

### 3.2.4 Quantifying entropy production

As noted in the introduction, the principal aim of our thermodynamic analysis is to calculate the entropy production within our ecosystem model. In the standard formulation of non-equilibrium thermodynamics, the entropy production  $\sigma_\alpha$  associated with a given flux  $F_\alpha$  ( $\alpha = R, W, AC, \dots$ ) is calculated as the product of that flux with a corresponding thermodynamic force  $X_\alpha$ , so that  $\sigma_\alpha = F_\alpha X_\alpha$ . Accordingly, we need to calculate the proper forces  $X_\alpha$  that are associated with each of the six fluxes  $F_\alpha$  in our ecosystem model.

The resource and waste exchange essentially describe a mixing process between two reservoirs A and B at different concentrations. The associated thermodynamic force can be directly calculated from the difference in the chemical potential  $\mu$  of these reservoirs via the relation  $X_{mix} = (\mu_A - \mu_B)/T$ , where  $T$  is the temperature [88]. For ideal solutions, the chemical potential scales with the logarithm of the concentration, i.e.  $\mu = \mu^r + RT \ln C$ , where  $R$  denotes the universal gas constant, and the superscript  $r$  refers to a reference state where the concentration  $C = 1$ . The resource and waste are approximated as ideal solutions, and as a result, we obtain<sup>3</sup>

$$X_R = (\mu_R^0 - \mu_R)/T = R \ln(C_R^0/C_R), \quad (3.12)$$

$$X_W = (\mu_W - \mu_W^0)/T = R \ln(C_W/C_W^0). \quad (3.13)$$

The abiotic and biotic fluxes  $F_{AC}$  and  $F_{BC}$  represent two parallel pathways of the same chemical transformation (3.3), which is the 'ecosystem metabolism'. Therefore, the thermodynamic force that is associated with these parallel transformations will be the same

$$X_{EM} = X_{AC} = X_{BC} \quad (3.14)$$

The thermodynamic force associated with a chemical reaction can be calculated from the relation  $X_{reac} = -A_{reac}/T$ , where  $A_{reac}$  denotes the affinity of the reaction, which is calculated from the difference in chemical potential between reaction products and reactants<sup>4</sup> [88]. Applying this procedure to reaction (3.3), we directly obtain

$$X_{EM} = R \ln(K_{eq} C_R/C_W), \quad (3.15)$$

where  $K_{eq}$  is the equilibrium constant introduced earlier.

Finally, we need to calculate the thermodynamic force associated with the synthesis of biomass (3.1) and the recycling of biomass back into resource (3.2). Applying the standard formalism of chemical thermodynamics to these reactions (3.1-3.2), the corresponding forces can be written as

$$X_{BS} = -(\mu_B - \mu_R)/T, \quad (3.16)$$

$$X_{BR} = -(\mu_R - \mu_B)/T \quad (3.17)$$

where  $\mu_B$  and  $\mu_R$  respectively denote the chemical potential of biomass and resource. One important observation is that both forces are exactly opposite (as must always be the case for opposite reaction pathways)

$$X_{BS} = -X_{BR} \quad (3.18)$$

Although theoretically valid, the expressions (3.16)-(3.17) need an explicit expression for the chemical potential of the biomass  $\mu_B$ . This poses clear problems in actual calculations. First of all, the biomass will be divided over different trophic compartments, and hence, one needs to calculate an 'averaged' chemical potential for this mix of various types of biomass. More fundamentally, to

<sup>3</sup>We assumed for simplicity that the reference chemical potentials of the resource (and similarly for the waste) are the same in both ecosystem and reservoir.

<sup>4</sup>The chemical potentials are 'weighted' with the stoichiometric coefficients, but these were taken unity in our description.

our knowledge, the issue of how to calculate the chemical potential for a population of living organisms has not yet been properly resolved. In other words, how to calculate the chemical potential of a tiger population at a certain biomass density, and how does this quantity differ from the chemical potential of a rabbit population at the same biomass density? Here, we will circumvent this difficulty by only considering the quasi steady state situation, where the  $\mu_B$  quantities will drop from the equations (as shown below). This 'trick' forms the cornerstone of our black box approach to the thermodynamic analysis of food webs.

Based on the above expressions for the thermodynamic forces, we are now able to list the entropy productions associated with all six fluxes

$$\sigma_R = F_R R \ln(C_R^0/C_R), \quad (3.19)$$

$$\sigma_W = F_W R \ln(C_W/C_W^0), \quad (3.20)$$

$$\sigma_{AC} = F_{AC} R \ln(K_{eq} C_R/C_W), \quad (3.21)$$

$$\sigma_{BC} = F_{BC} R \ln(K_{eq} C_R/C_W), \quad (3.22)$$

$$\sigma_{BS} = F_{BS} X_{BS}, \quad (3.23)$$

$$\sigma_{BR} = -F_{BC} X_{BS}. \quad (3.24)$$

Eqs. (3.19) and (3.20) are called the mixing EPs, due to diffusive processes. The other equations are reactive EPs, due to resource conversion, biomass synthesis and recycling. These expressions thus fully quantify all 'dissipation' that occurs within our model universe, where 'dissipation' is thus simply synonymous to 'entropy production'.

### 3.2.5 Two important entropy productions

Using these above expressions, two composite rates of entropy production can be derived that are of particular interest. Firstly, we can calculate the total entropy production that occurs *within the ecosystem alone*. Summation of the rates associated with the four internal fluxes (Fig. 3.1) results in

$$\sigma_{EM} \equiv \sigma_{AC} + \sigma_{BC} + \sigma_{BS} + \sigma_{BR}. \quad (3.25)$$

This quantity only accounts for the entropy production associated with the overall ecosystem functioning (the ecosystem metabolism), and is referred to as the 'ecosystem metabolism entropy production'. Secondly, we can calculate the total entropy production that occurs *within the complete model universe (both ecosystem and environment)*. Summation of all six entropy productions leads to

$$\sigma_{tot} \equiv \sigma_R + \sigma_{AC} + \sigma_{BC} + \sigma_{BS} + \sigma_{BR} + \sigma_W = \sigma_R + \sigma_W + \sigma_{EM}. \quad (3.26)$$

This quantity encompasses the dissipation that occurs internally within the ecosystem ( $\sigma_{EM}$ ), as well as the dissipation that results from the communication with the external surroundings (the mixing EP  $\sigma_R$  and  $\sigma_W$ ), and is referred to as the 'total entropy production' of the chemotrophic ecosystem.

### 3.2.6 Entropy balance formulation

The Second Law of Thermodynamics requires that for each independent flux  $F_\alpha$  the associated entropy production  $\sigma_\alpha$  should be positive [88]. A given flux

is 'independent' when it is not coupled to any of the other fluxes. In our model, five fluxes are independent ( $F_R$ ,  $F_W$ ,  $F_{AC}$ ,  $F_{RU}$  and  $F_{BR}$ ), and so the associated entropy productions should be positive. The flux  $F_{RU}$  was a coupling between  $F_{BS}$  and  $F_{BC}$  via the linkage of anabolism to catabolism as described in reaction (3.5) - see Fig. 3.1. The thermodynamic force of a linear combination of reactions is simply the linear combination of the forces of the individual reactions [88], and so the force associated with the coupled reaction (3.5) simply becomes

$$X_{RU} = qX_{BS} + (1 - q)X_{BC}. \quad (3.27)$$

In the case of coupling, the Second Law then requires that the overall entropy production of the coupled process (3.5) should be positive, i.e.,  $\sigma_{RU} > 0$ . Because  $F_{RU} = F_{BS}/q = F_{BC}/(q - 1)$ , one can easily verify that

$$\sigma_{RU} \equiv F_{RU}X_{RU} = \sigma_{BS} + \sigma_{BC} > 0 \quad (3.28)$$

Accordingly, we find that  $\sigma_{EM} > 0$  and  $\sigma_{tot} > 0$  because their individual components are all positive.

To provide further insight into the issue of entropy generation, we can write an entropy conservation equation for the model universe as a whole. We can always decompose the total entropy of the universe  $S_{uni}$  into separate contributions of ecosystem ('sys') and environment ('env'),  $S_{uni} = S_{env} + S_{sys}$ . The resulting entropy balance thus becomes

$$\frac{dS_{uni}}{dt} = \frac{dS_{env}}{dt} + \frac{dS_{sys}}{dt} = \sigma_{tot} \quad (3.29)$$

Because  $\sigma_{tot} > 0$ , equation (3.29) assures that the entropy of our model universe as a whole can only increase. No entropy export occurs because the universe is isolated as a whole.

### 3.3 (Quasi) steady state analysis

The EP expressions (3.19)-(3.24), the mass balances (3.6)-(3.8), and the entropy balance (3.29) are valid both in steady as well as transient regimes. Unfortunately, the inability to calculate the chemical potential of biomass  $\mu_B$  prevents the use of expressions to calculate the entropy production associated with food web operation. Here however, we will circumvent this difficulty by only considering the steady and quasi steady states, which refers to the situation where the properties of the ecosystem no longer vary with time. In the (quasi) steady state, the  $\mu_B$  quantities will drop from the equations (as shown below). This 'trick' forms the cornerstone of our black box approach to the thermodynamic analysis of food webs. For the moment, we assume that such a steady state can be reached (thus making abstraction of the possibility of oscillatory and chaotic dynamics). To make a distinction with transient properties, quasi steady state values are denoted with the superscript  $\times$  and steady states with the asterisk  $*$ .

#### 3.3.1 (Quasi) steady state mass and entropy balance

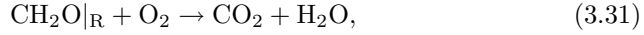
Because we treat the food web as a black box, we cannot say anything of its internal state. Yet, we do know that in a quasi steady state for the internal

biomass  $dC_B/dt = 0$ , eq. (3.8) directly results in

$$F_{BS}^\times = F_{BR}^\times \quad (3.30)$$

Combined with expression (3.18), this immediately reveals that  $\sigma_{BS}^\times = -\sigma_{BR}^\times$ , and so, there is no overall entropy production resulting from biomass synthesis and recycling. In the quasi steady state, the biotic concentration  $C_B$  is constant, or more generally, all biotic components in the food web are constant. This means that only the resource and waste concentrations  $C_R$  and  $C_W$  are left as variables.

Eq. (3.30) says that biomass synthesis should match the turn-over, and so the net metabolic activity of the food web only consists of respiration



which is nothing but the ecosystem metabolism. The quasi steady state ecosystem metabolism rate  $F_{EM}^\times$  is the combined result of the abiotic and biotic pathways of resource conversion (reaction (3.3)). Previously, we introduced the intrinsic time scale of the abiotic pathway as the inverse of the rate parameter  $\kappa_{AC}$  (which is constant) - see Eq.(3.9). To arrive at a similar time scale for the overall conversion of resources, we formally parameterize the quasi steady state ecosystem metabolism  $F_{EM}^\times$  as

$$F_{EM}^\times = \kappa_{EM}^\times (C_R - \frac{C_W}{K_{eq}}), \quad (3.32)$$

with  $\kappa_{EM}^\times$  an 'effective' quasi steady state rate parameter<sup>5</sup>, which is termed the *resource conversion rate parameter of the ecosystem*. This parameter generally is termed 'effective' because it result from a complex internal dynamics of the food web. It can be used as a master parameter when comparing the operation of different food webs in the (quasi) steady states. The inverse of  $\kappa_{EM}^\times$  specifies the time scale over which resources are degraded within the ecosystem. In a similar way, the parameter  $\kappa_{BC}^\times(C_B^\times) = \kappa_{EM}^\times - \kappa_{AC}$  is introduced as the quasi steady state *biotic resource conversion rate parameter of the food web*, and characterizes the time scale over which the food web converts resources.

The mass balance for the resource and waste now become

$$\frac{dC_R}{dt} = \alpha_R(C_R^0 - C_R) - \kappa_{EM}^\times(C_R - C_W/K_{eq}), \quad (3.33)$$

$$\frac{dC_W}{dt} = \kappa_{EM}^\times(C_R - C_W/K_{eq}) - \alpha_W(C_W - C_W^0). \quad (3.34)$$

The ecosystem metabolism EP in the quasi steady state simplifies to

$$\sigma_{EM}^\times = F_{EM}^\times R \ln(K_{eq} C_R^\times / C_W^\times), \quad (3.35)$$

Furthermore, the full steady state is obtained by dropping the temporal derivatives of the concentrations in the resource and waste balances (3.33) and (3.34). In that case, we find that the ecosystem metabolism rate and the exchange fluxes are related through

$$F_{EM}^* = F_{AC}^* + F_{BC}^* = F_R^* = F_W^* \quad (3.36)$$

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<sup>5</sup>Note that  $\kappa_{EM}^\times$  is not necessary a constant but might be dependent on the two variables  $C_R(t)$  and  $C_W(t)$ .

Combining the mass balance constraint (3.36) with expression (3.26) for the total entropy production, we eventually obtain

$$\sigma_{tot}^* = F_{EM}^* R \ln(K_{eq} C_R^0 / C_W^0) \quad (3.37)$$

This expression, as well as (3.35), does no longer contain the chemical potential of the biomass  $\mu_B$ , and so, we have circumvented the previously discussed difficulty of defining this quantity. The total entropy production depends on the external boundary conditions imposed upon the ecosystem (via  $C_W^0$  and  $C_R^0$ ), on the internal structure of the food web (via  $F_{EM}$ ) and on the internal state (via  $C_R$  and  $C_W$ ). Table 3.1 summarizes the different EP's and gives the restrictions on the states in order for them to become independent of explicit expressions for the biotic chemical potentials.

States	EP
all	Mixing EP
quasi steady states	Ecosystem metabolism EP
full steady	Total EP
none	EP of individual biological processes

Table 3.1: The states where the EP's are reliable because they do not explicitly depend on the biotic chemical potentials. Only the mixing EP is well defined in all states. On the opposite, the EP of individual biological processes (biomass synthesis, recycling) is always dependent on biotic chemical potentials, and therefore there are no states where these EP's are reliable.

Note that the term 'steady state' should be interpreted with caution: *the time invariance only applies to the ecosystem, and not the environment*. Accordingly, when applying the steady state condition to the entropy balance (3.29), only the term  $dS_{sys}/dt$  should vanish, and so one obtains

$$\frac{dS_{env}}{dt} = \sigma_{tot}^* > 0 \quad (3.38)$$

This equation illustrates that in the 'steady state', the properties of the environment should *not* remain constant in time. The assumption that  $C_W^0$  and  $C_R^0$  are fixed is nothing but a suitable approximation for large reservoirs with slow characteristic times (by the constraints of mass balance, the absolute mass of these external reservoirs should change in time). Effectively, the second law of thermodynamics requires that  $\sigma_{tot} > 0$ , and so the entropy balance (3.38) necessitates that the entropy of the environment should always increase. In other words, when the ecosystem resides within a steady state, all the entropy that is generated through interactions within the ecosystem or through interactions between ecosystem and environment, will ultimately 'accumulate' within the environment.

### 3.3.2 Ecosystems as far-from-equilibrium entities

One frequently encountered quote in texts on ecological thermodynamics is that 'ecosystems operate far-from-equilibrium'. However, a more precise quantitative interpretation of this 'distance from equilibrium' is typically not given. In

the classical interpretation, the far-from-equilibrium connotation refers to the thermodynamically 'improbable' state of living organisms [81]. In this view, organisms represent a highly self-organized form of matter, which resides in a low entropy state as compared to their surroundings. This intuitive idea can be formally expressed as

$$\Delta\mu = \mu_B - \mu_{ref}, \quad (3.39)$$

where  $\mu_{ref}$  denotes some reference potential, usually introduced as 'the chemical potential that biomass would have if it were brought in equilibrium with its surroundings' (e.g. [79]). Although intuitively appealing, there are two major problems with this definition. First, as explained above, a major roadblock in ecological thermodynamics is the impossibility to calculate the chemical potential  $\mu_B$  of an organism. This renders the definition (3.39) of little use in actual calculations. Second, and even more fundamentally, there is also a problem with the reference state. In real world situations, neither the ecosystem, nor the environment can reside in a state of thermodynamic equilibrium (see below). As a consequence, it is not possible to 'bring biomass in equilibrium with its surroundings', because the surroundings are not in thermodynamic equilibrium themselves. Consequently, there is no 'natural' equilibrium state that can serve as a logical reference to define  $\mu_{ref}$ .

A more meaningful interpretation of the distance from equilibrium is possible when looking at the disequilibrium between resource and waste products. For the chemotrophic ecosystems studied here, the term 'thermodynamic equilibrium' refers to the chemical equilibrium of the respiration reaction (3.37). Two situations can be distinguished, depending on whether thermodynamic equilibrium applies to the environment or to the ecosystem

$$\Delta\mu_{env} = \mu_R^0 - \mu_W^0 = RT \ln(K_{eq} C_R^0 / C_W^0), \quad (3.40)$$

$$\Delta\mu_{sys} = \mu_R^* - \mu_W^* = RT \ln(K_{eq} C_R^* / C_W^*). \quad (3.41)$$

Note that both these distances are defined in terms of abiotic state variables (i.e. resource and waste concentrations), and that they are expressed in units of energy. For convenience, we can also define corresponding quantities that are expressed in units of mass (by linearly expanding the logarithm in (3.40)-(3.41)). The mass-based analogue of  $\Delta\mu_{env}$  thus becomes

$$\Delta = C_R^0 - \frac{C_W^0}{K_{eq}}. \quad (3.42)$$

This quantity expresses how far the external environment is from thermodynamic equilibrium. In the vocabulary of non-equilibrium thermodynamics,  $\Delta$  is referred to as the 'thermodynamic gradient' that is imposed as a boundary condition upon the (eco)system. Obviously, the environment is in thermodynamic equilibrium when  $\Delta = 0$ . In a similar fashion, we can introduce a mass-based analogue of  $\Delta\mu_{sys}$  as

$$\delta = C_R^* - \frac{C_W^*}{K_{eq}}. \quad (3.43)$$

This quantity expresses the internal disequilibrium. In the limit  $\delta = 0$ , the waste is in equilibrium with the resource, but is the biomass also in equilibrium with

the resource? It is easy to show that the answer is affirmative: Using (3.27) with  $X_{BC} = X_{AC} = 0$  and  $X_{BS} = -X_{BR}$ , we get  $X_{RU} = -qX_{BR}$ . Furthermore,  $X_{RU} \geq 0$  and  $X_{BR} \geq 0$  because resource uptake and biomass recycling (turn-over) are spontaneous processes. And as  $q > 0$ , these forces should be zero. The latter means that  $\mu_B^* = \mu_R^* = \mu_W^*$ , so the system is in true internal equilibrium in this limit.

### 3.3.3 The ecosystem resource processing regime

If one specifies the steady state ecosystem metabolism  $F_{EM}^*$ , one can directly calculate the associated resource and waste concentrations from the mass balances (3.6)-(3.7) as

$$C_R^* = C_R^0 - F_{EM}^*/\alpha_R, \quad (3.44)$$

$$C_W^* = C_W^0 + F_{EM}^*/\alpha_W. \quad (3.45)$$

Upon substitution of these expressions into the kinetic parametrization (3.32), one directly finds that

$$F_{EM}^* = \frac{\kappa_{EM}^*}{1 + \kappa_{EM}^*/\kappa_{crit}} \Delta \quad (3.46)$$

where we have introduced the auxiliary rate constant

$$\kappa_{crit} = \left( \frac{1}{\alpha_R} + \frac{1}{\alpha_W K_{eq}} \right)^{-1} \quad (3.47)$$

The parameter  $\kappa_{crit}$  defines the characteristic time scale at which material is exchanged between ecosystem and environment. The value of  $\kappa_{crit}$  will be dominated by the rate limiting transfer. When  $\alpha_R \ll K_{eq}\alpha_W$  one obtains  $\kappa_{crit} \approx \alpha_R$ , and vice versa.

Expression (3.46) can be used to calculate  $F_{EM}^*$  from  $\kappa_{EM}^*$ , and vice versa. Accordingly, there are two equivalent ways to characterize the 'operation' of the ecosystem: either specifying  $F_{EM}^*$  or  $\kappa_{EM}^*$ . Here, we will employ the latter procedure. Effectively, we will use  $\kappa_{EM}^*$  as a master parameter that suitably summarizes the resource processing associated with a particular food web. When the value of  $\kappa_{EM}^*$  is known, one can directly calculate  $C_R^*$  and  $C_W^*$  through eqs. (3.44)-(3.46). From these concentrations, the disequilibrium distance  $\delta$ , the fluxes ( $F_{EM}^*$ ,  $F_R^*$  and  $F_W^*$ ) and entropy productions ( $\sigma_{EM}^*$ ,  $\sigma_R^*$  and  $\sigma_W^*$ ) can be subsequently calculated using the expressions of the previous sections. We will refer to this particular set of variables as the 'ecosystem resource processing regime' (ERPR). Note that in our analysis, we are not concerned with the internal details of the food web structure. The ERPR completely describes the overall effect of the food web on resource processing, but does not specify any 'internal' food web characteristics (biomasses, trophic flows). Effectively, the ERPR describes the operation of the food web in a black box fashion, and the parameter  $\kappa_{EM}^*$  epitomizes this black box approach.

## 3.4 Thermodynamic analysis of ecosystems

### 3.4.1 Physical environment and ecosystem state

Equipped with thermodynamic concepts and modeling tools introduced in the previous sections, we can now take up the actual thermodynamic analysis of ecosystems. Within a given fixed physical environment, there are - at least in theory - many ecosystem states that can be established. In order to be truly quantitative, we need a mathematical infilling of both the terms 'ecosystem state' and 'physical environment'. In the previous sections, these two terms were rigorously defined for our model universe.

Firstly, the specification of the 'physical environment' comes down to the specification of a set of six abiotic parameter values: the concentrations in the external resource reservoirs  $C_R^0$  and  $C_W^0$  (and so the thermodynamic gradient  $\Delta > 0$  is fixed), the transport coefficients  $\alpha_R$  and  $\alpha_W$ , the equilibrium constant  $K_{eq}$ , and the abiotic conversion parameter  $\kappa_{AC}$ . Secondly, as detailed above, each of these food webs will be associated with a certain ecosystem resource processing regime (ERPR). Moreover, this ERPR is completely determined when the value of resource processing parameter  $\kappa_{EM}^*$  is specified. In theory, the value of  $\kappa_{EM}^*$  can range from zero to infinity, and the ERPR of a natural food web will lie somewhere in between these two endpoints.

In the next sections, we will proceed in two steps. In a first step, we make no a priori judgement about the feasibility of a given food web, and we examine the behavior of all potential food webs within a given physical setting. To this end, we will scan the whole range  $0 < \kappa_{EM}^* < \infty$ , and in each point, we will calculate the corresponding solution of our ecosystem model<sup>6</sup>. In a second step, we then examine whether there are any special regimes within this range  $0 < \kappa_{EM}^* < \infty$  that are remarkable from a thermodynamic perspective.

### 3.4.2 Slow and fast food webs

As noted above, the rate constant  $\kappa_{crit}$  provides a characteristic time scale for the physical transport between ecosystem and environment. It also serves as threshold to distinguish between two types of ERPR, which we refer to as fast and slow food webs - see Fig. 3.2. When  $\kappa_{EM}^* \ll \kappa_{crit}$ , resource conversion is slow compared to the physical transport. In this scenario, the ERPR is said to be under 'reaction control' and the associated food web is categorized as 'slow'. Expression (3.46) reveals that  $F_{EM}^* \approx \kappa_{EM}^* \Delta$ , and so the ecosystem metabolism linearly scales with the resource processing parameter (note that the semi-logarithmic plotting in Fig. 3.2 obscures this linearity). As expected, under reaction control, the resource piles up within the ecosystem, while waste levels are low (Fig. 3.3). Oppositely, when  $\kappa_{EM}^* \gg \kappa_{crit}$ , resource conversion proceeds much faster than physical transport. In this scenario, the ERPR is said to be under 'transport control', and the associated food web is categorized as 'fast'. In this case, the ecosystem metabolism rapidly approaches a constant value  $F_{EM}^* \approx \kappa_{crit} \Delta$  when the resource processing rate parameter increases (Fig. 3.2). Under transport control, the resource is depleted by the high food processing activity within the food web, while waste levels are high (Fig. 3.3).

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<sup>6</sup>See [219] for the used values of the physical parameters

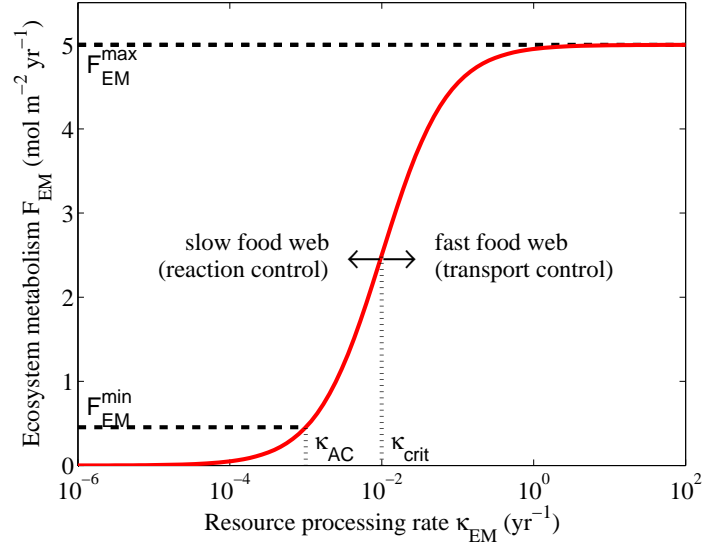


Figure 3.2: The ecosystem metabolism  $F_{EM}^*$  plotted as a function of the specific metabolic rate  $\kappa_{EM}^*$ .

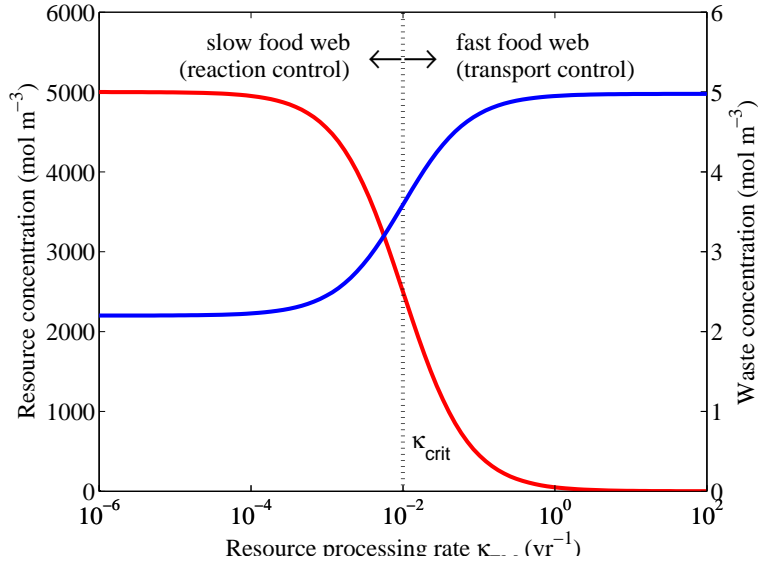


Figure 3.3: The resource  $C_R^*$  and waste  $C_W^*$  concentrations plotted as a function of the specific metabolic rate  $\kappa_{EM}^*$ .

When taken to the extreme, the slow and fast food webs give rise to two end-member situations. The 'minimal' end-member (or 'lazy' food web) is attained when there is no biological activity at all, and so  $\kappa_{EM}^* = \kappa_{AC}$ . The associated ecosystem metabolism becomes

$$F_{EM}^{min} = \frac{\kappa_{AC}}{1 + \kappa_{AC}/\kappa_{crit}} \Delta \quad (3.48)$$

As already indicated above, abiotic conversion of organic matter is typically slow. Therefore, in the limiting case where  $\kappa_{AC} \rightarrow 0$ , we find that  $F_{EM}^{min} \rightarrow 0$ . In this limit also, the resource and waste concentrations will simply match those of the external reservoirs, i.e.  $C_R^* = C_R^0$  and  $C_W^* = C_W^0$  (Fig. 3.3), and so, the distance from equilibrium becomes maximal and equals the thermodynamic gradient, i.e.  $\delta_{max} = \Delta$ .

On the opposite, the 'maximal' end-member (or 'crazy' food web) is attained when biological activity is very high: resources are frantically processed by the food web the moment they become available, and so  $\kappa_{EM}^* \rightarrow \infty$ . The associated ecosystem metabolism reaches a finite value

$$F_{EM}^{max} = \kappa_{crit} \Delta \quad (3.49)$$

In this limit  $\delta_{min} = 0$  and the ecosystem operates at internal thermodynamic equilibrium, i.e.  $\mu_R^* = \mu_B^* - \mu_W^*$ . Accordingly, when the rate constant  $\kappa_{EM}^*$  varies over the semi-infinite range,  $[0, \infty]$ , we find that the ecosystem metabolism  $F_{EM}^*$  varies over a finite range  $[0, F_{EM}^{max}]$ , and the corresponding disequilibrium distance  $\delta$  varies over the finite range  $[0, \Delta]$ .

### 3.4.3 Total and ecosystem entropy production

By scanning the full range  $0 < \kappa_{EM}^* < \infty$ , we have examined all possible resource processing regimes by food webs within a given physical environment. We can now examine whether among these many possible regimes, there are any 'remarkable' ones from a thermodynamic perspective. To this end, we can use Eqs. (3.35)-(3.37) to calculate the entropy productions  $\sigma_{EM}^*$  and  $\sigma_{tot}^*$  associated with a certain ERPR. These relations are plotted in Fig. 3.4. The characteristic shape of the two EP rates are very different. The  $\sigma_{tot}^*$  curve monotonically increases with increasing  $\kappa_{EM}^*$ . This contrasts strongly with the  $\sigma_{EM}^*$  curve, which starts at zero, goes through a maximum, and subsequently decreases again to zero.

In the expression for  $\sigma_{tot}^*$  the logarithmic factor remains constant, and so, the total EP simply scales with the ecosystem metabolism  $F_{EM}^*$ . The ecosystem EP  $\sigma_{EM}^*$  however shows a more complex dependence. Using the expressions (3.44)-(3.45) for  $C_R^*$  and  $C_W^*$ , it can be rewritten as

$$\sigma_{EM}^* = \frac{\kappa_{EM}^* \Delta}{1 + \frac{\kappa_{EM}^*}{\kappa_{crit}}} R \ln \left( \frac{K_{eq} \alpha_W}{\alpha_R} \frac{\alpha_R C_R^0 (1 + \kappa_{EM}^* / \kappa_{crit}) - \kappa_{EM}^* \Delta}{\alpha_W C_W^0 (1 + \kappa_{EM}^* / \kappa_{crit}) + \kappa_{EM}^* \Delta} \right). \quad (3.50)$$

The origin of the extremum in the  $\sigma_{EM}^*$  curve is explained by 'minimal' and 'maximal' end-member situations discussed above (assuming that abiotic conversion is very slow). In both end-members the EP  $\sigma_{EM}^*$  vanishes because the flux  $F_{EM}^*$  acts oppositely to the thermodynamic force  $X_{EM}^*$ . In the 'minimal' end-member (slow food web situation), the concentration difference between the internal ecosystem reservoirs is greatest (large but finite force), but the ecosystem's metabolism vanishes (zero flux). In contrast, the 'maximal' end-member, the ecosystem metabolism is maximal (large but finite flux), but concentration difference between the internal reservoirs vanishes (zero force). In both situations, the product of force and flux makes that  $\sigma_{EM}^*$  vanishes. In between the end-member regimes, the EP associated with ecosystem metabolism is positive, and hence, it should go through a maximum. This state of 'maximum

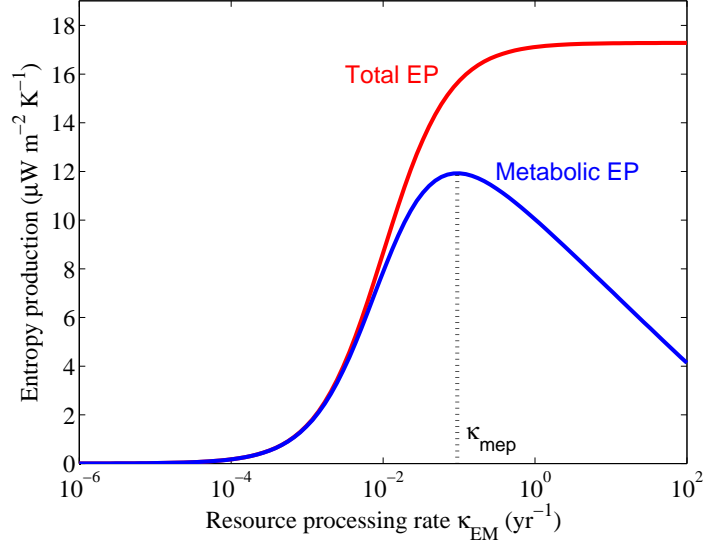


Figure 3.4: The total EP  $\sigma_{tot}^*$  and the ecosystem EP  $\sigma_{EM}^*$  as a function of the specific metabolic rate  $\kappa_{EM}^*$ .

ecosystem entropy production' (MaxEP) forms a third characteristic resource processing regime, and its associated metabolism is denoted  $F_{EM}^{MaxEP}$ . It is obtained by solving the non-linear equation  $d\sigma_{EM}^*/d\kappa_{EM}^* = 0$  where  $\sigma_{EM}^*$  is given by Eq.(3.50).

## 3.5 Discussion and conclusion

### 3.5.1 Ecological versus thermodynamic perspectives on food webs

The biological components within ecosystems interact with each other such that complex food webs emerge [186]. A fundamental question in ecology remains whether these food webs are shaped by (1) the interplay of internal interactions, or (2) external thermodynamic constraints, or (3) a combination of both. Up to now, the ecological literature has mainly explored the first option, looking at architecture, topology, complexity etc. - see review in [48]). In other words, the focus is on the *internal* organization of the food web, and the role of trophic interactions in this. Thermodynamics however offers a different, complementary perspective on food web functioning. Roughly speaking, one could say that ecological models primarily emphasize the 'inside' of the food web, and so, the abiotic environment receives a very crude description. In contrast, a thermodynamic approach focuses on the resource processing induced by the food web, and hence, it requires a detailed description of the communication with the 'outside' environment.

The analysis presented here takes this thermodynamic approach to the extreme: it makes abstraction of all internal details of the food web, and principally focuses on the interaction of the food web with the external surroundings. The

food web is essentially treated as a black box, represented by the resource processing constant  $\kappa_{EM}^*$ , which condenses all information on resource processing by the food web. This analysis in terms of  $\kappa_{EM}^*$  represents a generic way to assess the thermodynamic functioning of food webs. In a conventional food web model, one specifies a food web structure, and by doing this, one effectively selects a certain point along the axis  $0 < \kappa_{EM}^* < \infty$ . This way, our approach shows how traditional food web models can be cast within the formalism of non-equilibrium thermodynamics.

### 3.5.2 Conceptual problems in ecological thermodynamics

The idea that thermodynamic constraints could play a role in ecosystem development, has recently instigated considerable research into the use of thermodynamic principles in ecosystem analysis [79, 81]. Yet, some concerns have been issued about the quantitative rigor, the consistency, and the heuristic nature with which thermodynamic concepts are employed within ecological thermodynamics [108, 207, 52, 62]. Therefore, in our analysis, we devoted a lot of attention to derive reliable mathematical definitions of thermodynamic concepts (e.g. thermodynamic gradient, disequilibrium distance, entropy production, physical environment, ERPR) and to their correct translation into ecological terms. Every concept that was employed, was also defined in a quantitative sense.

Our analysis provides two clear examples of where past treatments of ecological thermodynamics have been confusing. A first issue is the often quoted statement that 'ecosystems are far-from-thermodynamic-equilibrium'. The classical interpretation of the distance from equilibrium is based on the difference in the chemical potential between biomass and some reference state. We show that this interpretation is troublesome, because (1) no procedure exists yet to define the chemical potential of biomass, and (2) no proper 'natural' reference state can be defined. To resolve this situation, we propose two alternative measures for the distance from equilibrium ( $(\Delta)$  and  $(\delta)$ ), which are based upon the disequilibrium between resources and waste products in respectively environment and ecosystem.

A second problem concerns the use of the term 'entropy production' in the context of ecological goal functions<sup>7</sup>. Such goal functions are extremal principles that - alone or in combination - predict ecosystem development [127]. In recent years, the notion of 'maximal entropy production' has surfaced a number of times in connection to ecological goal functions [61, 180]. Unfortunately, the term 'entropy production' has been always used without a proper definition of what this rate actually encompasses. In other words, it is not specified which interactions are included in the EP. Our analysis shows that such an unconstrained use of the term 'entropy production' is problematic. Multiple entropy productions can be defined, depending on what interactions are accounted for in the EP budget ( $\sigma_R$ ,  $\sigma_W$ ,  $\sigma_{AC}$ ,  $\sigma_{RU}$ , and  $\sigma_{BR}$  are the possible contributions in steady state for a simple ecosystem). These various entropy productions may show different extremal behavior.

<sup>7</sup>For a mathematical definition of goal function, see chapter 7.

## 3.6 The correspondence between ecological and climate systems

### 3.6.1 Entropy production as an ecological goal function?

Given previous propositions along this line [61, 180], it is logical to question whether EP serves as a useful ecological goal function? And if so, which EP should be maximal? Among the many possibilities, we have identified two entropy productions that could be relevant for ecosystem functioning: (a) the EP  $\sigma_{EM}^*$  associated with resource conversion within the ecosystem, and (b) the total EP  $\sigma_{tot}^*$  within both system and environment. Our analysis (Fig. 3.4) shows that only the ecosystem EP  $\sigma_{EM}^*$  has the proper mathematical form of a consistent goal function. The total EP  $\sigma_{tot}^*$  strictly increases with the resource conversion rate  $\kappa_{EM}^*$ , and hence, it does not show a maximum. In the real world, maximizing  $\sigma_{tot}^*$  would select a state of maximal resource processing that would have a finite value for  $\kappa_{EM}^*$ . However, any other monotonic function in  $\kappa_{EM}^*$  would select the same state, and therefore,  $\sigma_{tot}^*$  cannot be regarded a proper discriminatory goal function. In contrast, the metabolic EP  $\sigma_{EM}^*$  does show a clear maximum when the resource processing rate varies from zero to infinity.

Because  $\sigma_{EM}^*$  has the right mathematical form, this does not mean that the ecosystem EP also acts as a true ecological goal function. Whether  $\sigma_{EM}^*$  means something for ecosystem development, has to be verified from experimental observations on ecosystem functioning. The best way to test this maximum EP hypothesis, is by laboratory chemostat experiments (see previous chapter). A sample of 'dirty' water (containing a lot of organisms) is poured into the tank reactor to inoculate a complex food webs. When a steady state is reached, one can measure the total  $CO_2$  production rate, which should equal  $F_{EM}^*$ . Finally,  $\kappa_{EM}^*$  can be calculated by measuring the resource and waste concentrations, and this parameter can be compared with  $\kappa_{MaxEP}$ , the value where  $\sigma_{EM}^*$  reaches a maximum. For these experiments, it is important to check that the biota do not influence<sup>8</sup> the abiotic parameters  $\alpha_R$ ,  $\alpha_W$  and  $K_{eq}$ .

### 3.6.2 Maximum entropy production in the global climate system

The above discussion about EP as a goal function is related with the maximum entropy production (MaxEP) hypothesis used in e.g. climate modeling. The starting point of this MaxEP approach was due to work by Paltridge [150, 151], to understand the convective heat flows in the earth atmosphere. Paltridge's idea was to divide the model universe, containing the global atmosphere and oceans, in a number of compartments. The most simple formulation has four compartments (see fig. 3.5): the sun (at constant high temperature  $T_H^0$ ), the earth tropics (at variable temperature  $T_T$ ), the poles (at variable temperature  $T_P$ ) and interstellar space (at constant low temperature  $T_L^0$ ). The sun is radiating heat energy to the tropics, where it is transported to the poles by atmospheric (and oceanic) conduction and convection.

The dynamics are based on the energy balances of the tropics and pole

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<sup>8</sup>This influence is a priori possible and its relevance will become clear in chapter 8.

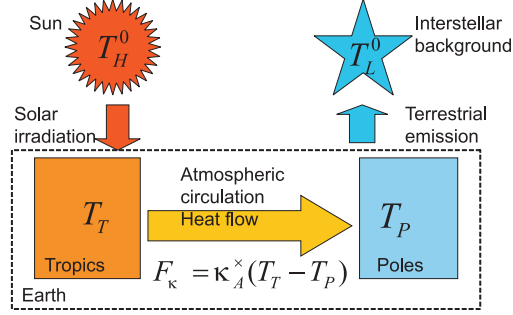


Figure 3.5: The climate system. The four compartments of Paltridge's model universe are shown, as well as the fluxes.

compartments:

$$\frac{dT_T}{dt} = \alpha_T(T_T^0 - T_T) - \kappa_A^x(T_T - T_P), \quad (3.51)$$

$$\frac{dT_P}{dt} = \alpha_P(T_P^0 - T_P) + \kappa_A^x(T_T - T_P), \quad (3.52)$$

with  $T_T^0$  and  $T_P^0$  the temperatures that the tropics and the poles would acquire in the absence of atmospheric heat transport<sup>9</sup> (they should not be confused with  $T_H^0$  and  $T_L^0$ ).  $\kappa_A^x$  is the effective atmospheric heat transport coefficient. The superscript  $\times$  indicates that this quantity is well defined in a quasi steady state for the atmosphere, i.e. a state whereby only  $T_T$  and  $T_P$  are variables, all other atmospheric quantities such as (average) wind velocity,... are constants. In these quasi steady states,  $\kappa_A^x$  will at most be dependent on the two variables, hence, the qualifier 'effective'. In this formulation, the climate is treated as a 'black box', without specifying the detailed inner structure and processes.

The atmospheric heat transport has EP (in the quasi steady state)

$$\sigma_A^x = \kappa_A^x(T_T - T_P) \left( \frac{1}{T_P} - \frac{1}{T_T} \right) \approx \frac{\kappa_A^x}{T_T^0 T_P^0} (T_T - T_P)^2, \quad (3.53)$$

which is the familiar product of the tropics-pole heat flow  $F_\kappa^x = \kappa^x(T_T - T_P)$ , and the equator-pole driving force (the temperature gradient). Maximizing this expression with respect to  $\kappa_A^x$  under the complete steady state conditions (with  $\alpha_T = \alpha_P$ ) gives

$$T_T^0 - T_{T,MaxEP}^* = \frac{T_{T,MaxEP}^* - T_{P,MaxEP}^*}{4} \quad (3.54)$$

and this result is close to the observed value. In other words,  $\kappa_A^x$  and  $F_\kappa$  of the atmosphere are not fixed, and these quantities apparently settle themselves

<sup>9</sup>To relate this formulation with the radiation systems described in section 2.4 and chapter 8, we can observe that the dynamics for  $T_T$  (in the absence of atmospheric heat transport), written as  $\frac{dT_T}{dt} = \alpha_{HT}(T_H^0)^4 - \epsilon_{LT}T_T^4$ , can be simplified to  $\frac{dT_T}{dt} \approx \alpha_T(T_T^0 - T_T)$  when  $T_T$  is close to  $T_T^0$ . Here,  $\alpha_T$  and  $\epsilon_T$  are the absorption and emission parameters for the tropics,  $\alpha_T \equiv 4\epsilon_{LT}(T_T^0)^3$  and  $T_T^0 \equiv \sqrt[4]{\frac{\alpha_{HT} + \epsilon_{LT}}{\epsilon_{LT}}} T_H^0$ .

in or close to a state of maximum EP for the atmospheric processes. This approach has been made more precise and extended to other planets or to vertical heat transport between the lower and the upper atmospheric layers [66, 86, 98, 145, 148, 209].

The similarity of this climate model and our four box ( $C_R^0$ ,  $C_R$ ,  $C_W$  and  $C_W^0$ ) chemotrophic ecosystem is obvious, as can be seen from fig. 1.4 (which is equivalent with 3.1) and fig. 3.5. The effective (quasi steady state) coefficients are resp.  $\kappa_A^\times$  and  $\kappa_{EM}^\times$ , and the above dynamics of  $T_T$  and  $T_P$  are equivalent with (3.33) and (3.34).

As the number of MaxEP observations and studies in planetary climate systems increases, and as there is such an intriguing correspondence between the 'black box' descriptions of both climate and ecosystems, one could examine whether MaxEP applies to ecosystems as well. We will come back to this issue in section 5.5 and chapter 10.

## Chapter 4

# Entropy production within classical ecological models: Lotka-Volterra revisited

### Abstract<sup>1</sup>

In order to describe ecological processes (biomass growth, decay, maintenance, predation, competition) from a thermodynamic perspective, we will study how to calculate the entropy production for generalized Lotka-Volterra systems. However, these classical models do not place enough emphasis on the exchange of resource and waste with the environment. Therefore, the generalized Lotka-Volterra systems are extended to include exchanges with environmental reservoirs of resource and waste compounds. This allows us to write the total steady state entropy production, and to compare this expression with other attempts in the literature concerning the unification of thermodynamics with Lotka-Volterra systems. The problems associated with some proposed 'entropy production' expressions are discussed, and it is shown that they do not always represent the production of thermodynamic entropy.

### 4.1 Introduction

In recent years, there have been a number of studies within the emerging discipline of 'thermodynamic ecology' that specifically address the issue of entropy production within 'traditional' ecological models, such as generalized Lotka-Volterra (LV) systems [32, 119, 120, 81]. There are however a number of problems associated with these approaches.

(1) Some of these studies advocate a different method for calculation of the EP. It is unclear how these individual definitions interrelate, and whether they are internally and mutually consistent.

(2) The advocated expressions are not derived from the standard theory of non-equilibrium thermodynamics, but are newly postulated 'ecological' definitions of EP. It is unclear how these new expressions relate to the classical definition of EP within non-equilibrium thermodynamics.

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<sup>1</sup>This chapter is based on an article in preparation.

Our analysis in chapter 2 and 3 has shown how one can apply the standard formulation of non-equilibrium thermodynamics to the analysis of ecosystems. This analysis was strictly 'orthodox': we restricted ourselves to the conventional definition of the entropy production rate and did not invoke any 'ecological' additions or modifications of the standard theory of chemical non-equilibrium thermodynamics [65, 88].

In chapter 3, the issue of the EP was treated in a generic fashion: the food web within the ecosystem was treated as a black box. Here, we provide an infilling of this black box, and consider explicit representations of the food web structure. An archetypal model representation of food webs are generalized Lotka-Volterra (LV) systems, which have been intensely studied in the field of theoretical ecology [30]. Accordingly, we will focus here on how to calculate the EP within these LV systems. One problem that immediately arises with a thermodynamic analysis of LV systems, is that classical LV models do not account for communication with the environment (i.e. mass and energy exchange). In other words, organisms grow on certain resources, but the origin and fate of these resources are not explicitly modeled. As shown in detail in chapter 3, the environment plays a crucial role in calculating the EP. To resolve this, we will first extend the LV model description with suitable exchange terms with the environment (like in a chemostat dynamics [185]). Both chemostat and LV dynamics are thus combined into a generalized LV chemostat dynamics, for which we will write down the correct mathematical expression for the EP rate. The original LV system will be obtained as a limiting case of our extended LV system, and hence the EP in this limit can be compared with EP expressions that have been proposed in the LV literature [32, 119, 120, 81]. Our conclusion will be that the published mathematical expressions in [32, 119, 120, 81], although they are termed 'the entropy production', have no link with the thermodynamic EP, or they correspond with the thermodynamic EP only in a rather restricted limiting case. At best, they define a set of novel ecosystem properties. Whether these quantities are relevant for ecosystem functioning or ecosystem development remains an open question.

## 4.2 The generalized Lotka-Volterra chemostat dynamics

To construct the generalized Lotka-Volterra chemostat dynamics, we will first look at the different processes and the associated fluxes (rates). The model forms an idealization of a chemotrophic ecosystem. The food web that is present within the ecosystem ultimately thrives on a single food resource  $R$  (e.g. glucose), and the metabolic processing of this resource eventually results in the metabolic end-product or "waste"  $W$  (e.g. the  $CO_2$  liberated in respiration). Both resource and waste are exchanged with the environment at the respective rates

$$F_R = \alpha_R(C_R^0 - C_R) \quad (4.1)$$

and

$$F_W = \alpha_W(C_W - C_W^0), \quad (4.2)$$

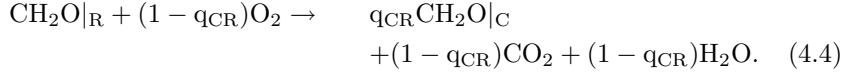
where  $C_R^0$  and  $C_W^0$  are the (fixed) concentrations of reservoirs in the environment. These exchanges are similar to those of a chemostat dynamics (see fig. 2.1).

Apart from these two exchanges, there is a third abiotic process, the abiotic conversion from resource to waste is given by the oxidation reaction (3.3), with abiotic conversion rate

$$F_{AC} = \kappa_{AC}(C_R - C_W/K_{eq}). \quad (4.3)$$

The food web itself consists of  $B$  different types of organisms (species). Each species can have two trophic interactions: (1) feeding on the abiotic resource  $R$  (i.e. abiotic resource consumption), or (2) preying on another species in the food web (i.e. predation). These two trophic interactions are now described separately.

Let us first consider a primary consumer species (index  $C$ ) whose biomass is written in the same stoichiometry as the resource, i.e. in units of  $\text{CH}_2\text{O}|_C$  (which is a good approximation for e.g. algae [188]). The consumer biomass concentration<sup>2</sup> is  $C_C$ . The uptake of resource and the associated growth (synthesis) of biomass is modeled by the transformation (see eq. (3.5))

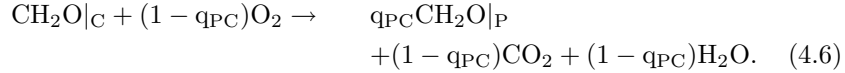


The parameter  $q_{CR} < 1$  is the consumer's yield factor for growth on the resource, which is now treated as a constant. The rate of reaction (4.4) is termed the rate of growth of the consumer feeding on the resource, and is given by the kinetic expression

$$F_{gCR} = g_{CR}(C_R - C_W/K_{eq})C_C, \quad (4.5)$$

where the growth rate parameter<sup>3</sup>  $g_{CR}$  is a positive constant. Expression (4.5) is a classical linear functional response (Holling type I [72], i.e. bilinear in  $C_R$  and  $C_C$ ), but for the extra addition of the  $-C_W/K_{eq}$  term. This term is added for thermodynamic consistency: the growth rate should vanish at thermodynamic equilibrium, as was the case for the abiotic conversion of resource - see eq. (4.3)<sup>4</sup>

The growth of a predator  $P$  feeding on a prey-consumer species  $C$  is described in a similar way as (4.4):




---

<sup>2</sup>This is not the concentration of individual consumer organisms. It is rather the concentration of biomass *units* (elementary building blocks) in all the consumer individuals. We can write the concentration of consumers as  $C'_C = C_C/a_C$ , with  $a_C \gg 1$  the average number of basic building blocks (which is equivalent with the number of carbon atoms in the above example) in one organism.

<sup>3</sup>Most ecological models take the growth rate in terms of the concentration of organisms. This can be done by replacing  $g_{CR}C_C \rightarrow g'_{CR}C'_C$ , with  $g'_{CR} = a_C g_{CR}$  the growth rate parameter studied in most ecological models.

<sup>4</sup>This term will also be derived by other means in chapter 7. We could also implement other growth kinetics, such as a Monod (Holling type II) dependence on the resource. Such more complex descriptions are not explored here, as they lead to more intricate mathematical expressions.

where  $\text{CH}_2\text{O}|_P$  is stoichiometric representation of the predator biomass. The associated rate of growth of the predator feeding on the consumer is given by

$$F_{gPC} = g_{PC}C_C C_P. \quad (4.7)$$

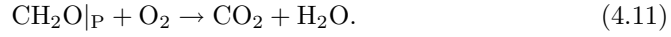
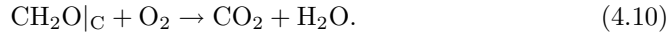
In this,  $C_P$  is the predator biomass density,  $q_{PC} \leq 1$  denotes the predator's yield of living on the consumer, and  $g_{PC}$  is the associated growth rate parameter.

Each species can also lose biomass in two different ways : (1) the conversion (turn-over) of biomass back into resource  $R$ , or (2) the metabolic conversion of biomass into waste products  $W$ , by basal maintenance. The biomass decay due to turn-over is described via the transformations



Biomass turn-over thus means that biomass simply disassembles (recycles) into basic building blocks, which become again available for biomass synthesis or respiration. It is associated with death by e.g. disease, accident or aging.

The biomass decay due to basal maintenance (the energetic 'cost' to stay alive) is described by the maintenance respiration:



Basal maintenance represent a complete oxidation (burning) of biomass to waste. Turn-over biomass decay is given by the simple first-order kinetics<sup>5</sup>

$$F_{tC} = r_C d_C C_C, \quad (4.12)$$

$$F_{tP} = r_P d_P C_P, \quad (4.13)$$

where the total decay rate parameters  $d_C$  and  $d_P$  and the recycling ratios  $r_C \leq 1$  and  $r_P \leq 1$  are positive constants. The maintenance biomass decay for consumer and predator reads

$$F_{mC} = (1 - r_C) d_C C_C, \quad (4.14)$$

$$F_{mP} = (1 - r_P) d_P C_P. \quad (4.15)$$

The total disappearance rate is composed of the above two parts:  $F_{dC} = F_{tC} + F_{mC}$ .

To simplify the notion for the complete generalized LV chemostat dynamics, let us write all biota as  $C_b$ , with the index  $b = 1, \dots, B$  indexing the different species. Implementing the relations (3.3)-(4.15) into the associated mass balance equations, the resulting dynamics of the ecosystem becomes

$$\frac{d}{dt}C_R = F_R - F_{AC} - \sum_b (F_{gbR} - F_{tb}), \quad (4.16)$$

---

<sup>5</sup>Note that higher order terms might be required, especially in the Lotka-Volterra limit  $\alpha_R \rightarrow \infty$  (see later), because otherwise the steady state biomass concentration becomes infinite in this limit. In our formalism, this implies that e.g.  $d_C$  is an increasing function of  $C_C$ . We will not study such extensions here.

$$\frac{d}{dt}C_b = q_{bR}F_{gbR} - \sum_{b'}(F_{gb'b} - q_{bb'}F_{gbb'}) - F_{tb} - F_{mb}, \quad (4.17)$$

$$\begin{aligned} \frac{d}{dt}C_W &= -F_W + F_{AC} + \sum_b(1 - q_{bR})F_{gbR} \\ &\quad + \sum_{bb'}(F_{gb'b} - q_{bb'}F_{gbb'}) + \sum_b F_{mb}, \end{aligned} \quad (4.18)$$

or explicitly

$$\begin{aligned} \frac{d}{dt}C_R &= \alpha_R(C_R^0 - C_R) - (\kappa_{AC} + \sum_b g_{bR}C_b)(C_R - C_W/K_{eq}) \\ &\quad + \sum_b r_b d_b C_b, \end{aligned} \quad (4.19)$$

$$\begin{aligned} \frac{d}{dt}C_b &= q_{bR}g_{bR}(C_R - C_W/K_{eq})C_b \\ &\quad - \sum_{b'}(g_{b'b} - q_{bb'}g_{bb'})C_b C_{b'} - d_b C_b, \end{aligned} \quad (4.20)$$

$$\begin{aligned} \frac{d}{dt}C_W &= \alpha_W(C_W^0 - C_W) + (\kappa_{AC} + \sum_b(1 - q_{bR})g_{bR}C_b)(C_R - C_W/K_{eq}) \\ &\quad + \sum_{bb'}(g_{b'b} - q_{bb'}g_{bb'})C_b C_{b'} + \sum_b(1 - r_b)d_b C_b. \end{aligned} \quad (4.21)$$

This way, we basically obtain the population dynamics of a model that incorporates chemostat-type exchanges of resource and waste and Lotka-Volterra-type predator-prey interactions (Smith and Waltman 1995). This 'extended' equation set can be easily reduced to the classical generalized LV equations. To this end, let us define the auxiliary parameters

$$\epsilon_b \equiv q_{bR}g_{bR}(C_R - C_W/K_{eq}) - d_b, \quad (4.22)$$

$$\gamma_{bb'} \equiv g_{b'b} - q_{bb'}g_{bb'}. \quad (4.23)$$

When taking the 'LV limit'  $\alpha_R \rightarrow \infty$  and  $\alpha_W \rightarrow \infty$ , we obtain approximately constant resource and waste concentrations  $C_R \approx C_R^0$  and  $C_W \approx C_W^0$ . We are left with a generalized LV dynamics (generalizing the predator-prey LV)

$$\frac{d}{dt}C_b = C_b(\epsilon_b - \sum_{b'} \gamma_{bb'} C_{b'}). \quad (4.24)$$

Here,  $\epsilon_b$  represents the inherent growth rate of species  $b$ , i.e. the growth minus the death in the absence of all other species. The interaction matrix  $\gamma_{bb'}$  represents the effect of species  $b'$  on the population growth rate of  $b$ .

As we focus on the derivation of the mathematical expression for the EP, we will not study the solutions of the above dynamics<sup>6</sup>.

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<sup>6</sup>To guide the reader, we mention that chapter 6 discusses the (steady state) solutions of a generalized LV chemostat ecosystem with one resource, one consumer and one omnivore (the RCO model), chapter 7 studies the solutions of the resource-consumer-predator (RCP) ecosystem and chapter 8 studies the RC model with variable exchange rate ( $\alpha_R$  dependent on the biota).

### 4.3 Entropy production rates

As extensively discussed in chapter 2, a fundamental problem in thermodynamic ecology is that we cannot calculate EP rates in a transient state. The problem is that we cannot attribute chemical potentials to the organisms of the ecosystem, and hence, it is not possible to define suitable thermodynamic forces for the biological transformations that are catalyzed by the food web. However, we have shown that it is possible to derive EP rates when the ecosystem resides in steady state. For the EP associated with the ecosystem metabolism, we obtained

$$\sigma_{EM}^* = \alpha_R(C_R^0 - C_R^*)R \ln \frac{C_R^* K_{eq}}{C_W^*} = F_{EM}^* X^*. \quad (4.25)$$

The factor

$$X^* = R \ln \frac{C_R^* K_{eq}}{C_W^*} \quad (4.26)$$

is the 'internal' driving force, and

$$F_{EM}^* = (\kappa_{AC} + \sum_b g_{bR} C_b^*)(C_R^* - C_W^*/K_{eq}) - \sum_b r_b d_b C_b^* \quad (4.27)$$

is the ecosystem metabolism flux in the steady state. This flux is the sum of an abiotic part and biotic parts:

$$F_{EM}^* = \kappa_{AC}(C_R^* - C_W^*/K_{eq}) + \sum_b F_b^*, \quad (4.28)$$

with

$$F_b^* = \left( \frac{\epsilon_b^* + d_b}{q_{bR}} - r_b d_b \right) C_b^*. \quad (4.29)$$

Therefore, we can write the biotic part of the ecosystem metabolism EP as the bilinear form of fluxes and forces:

$$\sigma_{bio}^* = \sum_b F_b^* X_b^*, \quad (4.30)$$

whereby every force  $X_b^*$  equals  $X^*$ . Finally, we can take the LV limit ( $\alpha_{R,W} \rightarrow \infty$ ). In this limit,  $\epsilon_b^*$  becomes  $\epsilon_b^0 = q_{bR} g_{bR} (C_R^0 - C_W^0/K_{eq}) - d_b$  and  $X^*$  becomes  $X^0 = R \ln(C_R^0 K_{eq}/C_W^0)$ . The latter is the overall driving force, determined by the environment. That means that in the LV limit, the EP associated with the ecosystem metabolism equals the total EP of the model universe. This total EP is the sum of the mixing EP (due to the exchanges of the resource and the waste between ecosystem and environment) and the ecosystem metabolism EP. In other words, in the LV limit there is no mixing EP associated with the exchanges of resource and waste with the environment. To explain this property, note that the driving force for e.g. the resource exchange is given by  $X_R = R \ln(C_R^0/C_R)$ , and in the LV limit this driving force becomes zero. The conjugate flux  $F_R$  however remains finite, and hence the product  $\sigma_R = F_R X_R$ , the mixing EP, becomes zero.

## 4.4 Discussion: a comparison of entropy production expressions

The thermodynamically correct EP expression (4.30) (with (4.29)) of a generalized LV system can be compared with previous expressions that have been proposed in the literature. The major advantage of these previous attempts is that they are not always restricted to the steady states<sup>7</sup>. However, they have several important drawbacks:

- the ecosystems are often coupled with only one environment, instead of two environmental reservoirs,
- the abiotic components (e.g. resource and waste) and the exchanges between the system and the environment are often not taken into account, although biotic components can have a strong influence on them<sup>8</sup>,
- in some cases, not all relevant reactions are taken into account in the EP expression,
- the expressions for the thermodynamic forces and fluxes are usually rather postulated 'ad hoc', so the resulting EP expressions are not equivalent with our expressions, which were derived by classical irreversible thermodynamics (as was done in chapters 2 and 3).

Let us discuss five EP proposals.

### 4.4.1 Chakrabarti-Ghosh-Bhadra

Chakrabarti, Ghosh and Bhadra (CGB) [32] provided the first attempt to calculate the EP associated with LV dynamics. They started from a force-flux EP expression of non-equilibrium thermodynamics  $\sigma = \sum_b F_b X_b$ . Subsequently however, these authors employed non-standard interpretations for the flows and fluxes. The 'CGB' forces were defined as the difference in the population density with reference to the steady state of the LV dynamics  $X_{b,CGB} = N_b^* - N_b$  (where \* denotes the steady state of the LV dynamics (4.24) and  $N_b$  measures the biomass in appropriate units), because the authors stated that in this way  $X_b$  acts as a driving force. There is potential for some confusion here, because  $X_b$  indeed acts as a driving force towards the steady state, but it is not the thermodynamic driving force because the latter acts towards thermodynamic equilibrium (with typically  $N_b^{eq} = 0$ ). The 'CGB' flows were defined as the changes in the logarithm of the biomass,  $F_{b,CGB} = \frac{d \ln N_b}{dt}$ , because in this way there is a linear phenomenological relation

$$F_{b,CGB} = \sum_{b'} \gamma_{bb'} X_{b',CGB}. \quad (4.31)$$

This relation is however unrelated with Onsager's work on linear response [146] (see (5.1) in chapter 5). The latter only works when the system is close to equilibrium, but a LV system is thermodynamically far from equilibrium. Further comments can be made on the choice of variables  $N_b$ . They are basically the

<sup>7</sup>In chapter 7 we will study the EP for a RCP model in both steady *and transient* states. But that approach is plagued with some intricacies.

<sup>8</sup>Take e.g. the resource exchange  $F_R$ . It depends on the resource concentration  $C_R$ , and as the resource is depleted by the consumers, these biota can have some influence on the exchanges.

concentrations  $C_b$  measured in appropriate energy units (J/K). But how this change of units should be done is not clear, because the free energies (and hence the chemical potentials) of the biological species should be known. According to the authors, the biotic chemical potentials are  $\mu_b/T = N_b^* - N_b$ , but they did not give clear arguments for this.

To summarize, the EP expression used by Chakrabarti et al.,

$$\sigma_{CGB} = \sum_b (N_b^* - N_b) \left( \frac{d \ln N_b}{dt} \right), \quad (4.32)$$

has some major drawbacks. As it stands like this, it cannot describe the total EP, because in the non-equilibrium steady state(s) the above 'CGB' forces and fluxes are zero, resulting into a vanishing EP. But the thermodynamic EP (4.30) is definitely not zero in non-equilibrium (steady) states.

#### 4.4.2 Michaelian

Another proposition was made by Michaelian [120]. The basic assumption made by Michaelian is that the ecosystem entropy is a well defined function of the biomass concentrations (the populations), and of no other variables:  $S = S(C_b)$ . Then we can write for the entropy change

$$\begin{aligned} \frac{dS}{dt} &= \sum_b \frac{\partial S}{\partial C_b} \frac{dC_b}{dt} \\ &= \sum_b \left( \Gamma_b + \sum_{b'} \Gamma_{(bb')} C_{b'} \right) C_b. \end{aligned} \quad (4.33)$$

with  $\Gamma_b = -\epsilon_b \nu_b / T$  and the symmetrized matrix  $\Gamma_{(bb')} \equiv \frac{\Gamma_{bb'} + \Gamma_{b'b}}{2} = \gamma_{bb'} \nu_b / T = \gamma_{b'b} \nu_{b'} / T$ . The 'biological potential'  $\nu_b = -T \partial S / \partial C_b$  is the analogue of the chemical potential for the biomass concentration of species  $b$ . The above expression for the entropy change is basically a second order approximation in a series expansion. According to Michaelian, the first order term with  $\Gamma_b$  represents the EP due to "one-body irreversible processes occurring within the individual, such as photosynthesis, evapotranspiration, respiration, metabolism, etc." Similarly, the second order term with  $\Gamma_{bb'}$  involves the EP of two-body interactions between individuals (predation, competition, symbiosis, etc.). Higher order terms (n-body interactions) are ecologically less relevant (except for societies).

Let us now comment on Michaelian's approach. First, the above expression is not the entropy *production*, but rather the entropy *change* of the ecosystem. Consequently, the above expression (4.33) becomes zero in a steady state instead of in thermodynamic equilibrium. Secondly, the basic assumption is dubious: there is no guarantee that the entropy is simply a function of the populations. Related with this, Michaelian derived the biological potentials  $\nu_b$ , whereas these are exactly the quantities which were shown to be 'tricky' and possibly not well defined, see the discussion in chapter 2. Furthermore, these biological potentials (if they exist), and hence also the  $\Gamma$ 's, cannot be treated as constants, because that leads to a thermodynamic inconsistency. Close to equilibrium, there is a very small force<sup>9</sup>  $X_{b,M} = C_b$ . But in this regime, there should be a linearity between forces and fluxes [146]. As the 'Michaelian' fluxes were given by

<sup>9</sup>Note that Michaelian took the force  $X_{b,M}$  simply equal to  $C_b$ , which might seem strange

$F_{b,M} = \Gamma_b + \sum_{b'} \Gamma_{(bb')} C_{b'}$ , thermodynamic consistency requires  $\Gamma_b \rightarrow 0$ . If  $\Gamma_b$  was constant, it would also vanish far from equilibrium, deleting the EP contributions from one-body interactions. This would indicate that photosynthesis, respiration,... all are reversible, non-dissipative processes.

#### 4.4.3 Jørgensen-Svirezhev

In the book by Jørgensen and Svirezhev (JS) [81], different expressions for the EP were given. We will discuss three of them.

##### Jørgensen-Svirezhev 1

On page 148 one can read an expression for the EP as a bilinear form of forces and fluxes:

$$\sigma_{JS1} = \sum_b \left( \ln \frac{C_b}{C_b^*} \right) \left( \frac{dC_b}{dt} \right). \quad (4.34)$$

This EP is also used in [190], and it is an expression very similar to the one used by Chakrabarti et al., with a similar line of reasoning for its derivation. One can formulate the same objections as in subsection 4.4.1.

##### Jørgensen-Svirezhev 2

On page 165 in [81], one can read

$$T\sigma_{JS2} = \sum_b d_b N_b, \quad (4.35)$$

with  $d_b$  the decay rate. This expression can be derived from (4.30-4.29) by imposing some restrictions:

- The system is in the steady state,
- there is no recycling (all  $r_b = 0$ ),
- all the yields are unitary  $q_{bR} = q_{bb'} = 1$  and
- the ecosystem is a *trophic chain* (only one species at each trophic level), i.e. the  $\gamma$ -matrix has the form

$$\gamma = \begin{pmatrix} 0 & \gamma_{12} & 0 & 0 \\ -\gamma_{12} & 0 & \gamma_{23} & 0 \\ 0 & -\gamma_{23} & 0 & \gamma_{34} \\ 0 & 0 & -\gamma_{34} & \ddots \end{pmatrix}$$

The  $N_b$  obtain the appropriate units by writing them as  $N_b^* \equiv C_b^* T X^*$ . Using (4.30), together with (4.29), we can write

$$T\sigma_{bio}^* = g_{1R}(C_R^* - C_W^*/K_{eq})N_1^*, \quad (4.36)$$

---

and all too simple. However, there is some arbitrariness in the definition of the forces and the fluxes. Only the product is not arbitrary.

whereby the index 1 refers to the lowest trophic level: the primary consumer which is directly feeding on the resource  $R$ . Under the steady state conditions, it is easy to verify that the above expression becomes

$$T\sigma_{bio}^* = \sum_b d_b N_b^*, \quad (4.37)$$

which equals  $T\sigma_{JS2}^*$ .

Although we have obtained the correct expression, we can give some remarks:

- The restriction of unitary yields  $q_{bR} = q_{bb'} = 1$  is ecologically rather meaningless, because they imply that the organisms have maximal growth efficiency, i.e. there is no respiration (production of waste  $W$ ) associated with the biomass synthesis of the organisms.
- The steady state condition was not clearly mentioned in [81]. The expression is not true in transient states, because then not all EP producing reactions (e.g. due to growth) are taken into account. Only biotic decays are used, and these terms equal the growth rate  $g_{1R}(C_R^* - C_W^*/K_{eq})N_1^*$  only in a steady state.
- The relation between  $N_b$  and  $C_b$  was not clearly mentioned in [81]. The biomass  $N_b$  should be measured in appropriate energy units, but this implies knowledge of the forces  $X$ , or the chemical potentials.

The latter remark, the disregard of the forces, is also applicable to EP discussions in the work by e.g. Aoki [5, 6] and Ludovisi et al. [102]. In these studies, the EP due to metabolic respiration is discussed, but it is presented as the respiration rate, neglecting the conjugate thermodynamic forces. These conjugate forces generally depend on the ecosystem variables, and therefore they should not be treated as constants. It is only in the total steady state EP that the force is the external driving force, which is independent of the ecosystem variables.

### Jørgensen-Svirezhev 3

As a third proposal, at page 201 of [81], one can read

$$T\sigma_{JS3} = \sum_{bb'} \gamma_{bb'} N_b N_{b'}, \quad (4.38)$$

with the  $N_b$  variables again in appropriate units. It is easy to see that this is the correct biotic thermodynamic EP expression (4.30) when a number of conditions are satisfied:

- The system is in the steady state,
- all recycling ratio's are  $r_b = 1$  and
- all yield factors of the primary consumers are  $q_{bR} = 1$ .

The  $N_b^*$  now obtain the appropriate units by writing  $N_b^* \equiv \sqrt{TX^*} C_b^*$ . We now obtain the EP in the correct units:

$$\sigma_{JS3}^* = \sum_{bb'} \gamma_{bb'} C_b^* C_{b'}^* X^*. \quad (4.39)$$

(Note that eq. 4.39 is a similar expression as used by Michaelian for  $\Gamma_b = 0$ .)

In the LV limit,  $X^*$  becomes  $X^0$ . As discussed in [81], in this LV limit and when  $\gamma_{bb'}$  is symmetric, this EP (4.39) is maximum under the 'constant biomass' constraint:  $\sum_b C_b$  constant, or with (4.24)

$$\sum_b \epsilon_b C_b X^0 = \sum_{bb'} \gamma_{b'b} C_{b'} C_b X^0 = \sigma_{JS3}. \quad (4.40)$$

Let us briefly derive this maximum EP principle<sup>10</sup>. The line of reasoning is not influenced by taking  $X^0 = 1$ . Write the Lagrangian as

$$L = \sum_{bb'} \gamma_{b'b} C_{b'} C_b + \lambda \left( \sum_b \epsilon_b C_b - \sum_{bb'} \gamma_{b'b} C_{b'} C_b \right), \quad (4.41)$$

with  $\lambda$  a Lagrange multiplier that settles the constraint. We can now take the extremum  $\partial L / \partial C_b$ , which should be zero. Or by summing

$$\sum_b C_b \frac{\partial L}{\partial C_b} = 2 \sum_{b'} \gamma_{b'b} C_{b'} + \lambda (\epsilon_b - 2 \sum_{b'} \gamma_{b'b} C_{b'}) = 0. \quad (4.42)$$

When  $\lambda = 2$ , this becomes nothing but our constraint. Therefore, consistency allows us to take  $\lambda = 2$ , and the reduced Lagrangian becomes

$$\bar{L} = 2 \sum_b \epsilon_b C_b - \sum_{bb'} \gamma_{b'b} C_{b'} C_b. \quad (4.43)$$

Taking the extrema again, we see that  $\partial \bar{L} / \partial C_b = 0$  gives the steady state conditions. In other words, the extremum of  $\sigma_{JS3} = \sum_{bb'} \gamma_{b'b} C_{b'} C_b$  under the constant biomass constraint is equivalent with the steady state.

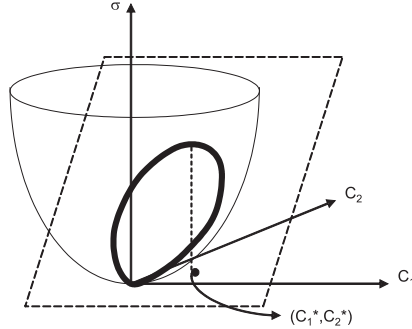


Figure 4.1: The maximum EP principle by Jørgensen and Svirezhev, for two competing biotic species  $C_1$  and  $C_2$ .

Fig. 4.1 shows the EP for two variables  $C_1$  and  $C_2$ . The symmetry of  $\gamma$  means that these two species are primary consumers in 'indirect' competition

<sup>10</sup>Note that [81] erroneously stated that this EP attained a *minimum*, postulating an ecological counterpart of Prigogine's minimum EP principle [88]. Also a minimum EP principle was claimed for the trophic chain ecosystem, using  $\sigma_{JS2}$ , but we can show that that proof contains some error. An elaboration on that point would deviate us too much from our storyline. The conclusion should be that the trophic chain and the trophic level do not obey a minimum EP principle.

for the resource, or in symmetric direct competition (e.g. death by fighting). In other words, under the above set of restrictions, and when there is symmetric competition on the first trophic level, the EP becomes a quadratic potential and the constraint is a tilted plane. The intersection is an ellipse, and the maximum value gives the steady state.

However, this maximum EP principle is simply a mathematical curiosity, without much experimental relevance, due to several reasons:

- The 'constant biomass' constraint is not necessarily applicable in the LV dynamics. Transient states of the LV system do not necessarily obey biomass conservation. This means that we do not observe an increase in EP  $d\sigma/dt \geq 0$  under ecosystem evolution<sup>11</sup>. Furthermore, the EP expression  $\sigma_{JS3}$  is only valid in a steady state. Outside a steady state, the 'thermodynamic entropy production' deviates from this 'JS entropy production':  $\sigma \neq \sigma_{JS3}$ . Therefore, this principle is better called 'maximum JS entropy production' instead of 'maximum entropy production'.
- The symmetry of  $\gamma_{bb'}$  means that this maximum EP principle does not work for e.g. consumer-predator interactions.
- The restrictions such as unitary yields  $q_{bR} = 1$  are ecologically meaningless, because the primary consumers do not have maximal growth efficiency.

## 4.5 Summary

In this chapter we have carried out a critical evaluation of the various forms that have been proposed for the EP rate in ecological models. This is done for the case of generalized Lotka-Volterra models in chemotrophic ecosystems. We have first derived an expression (4.25) for the EP in generalized LV chemostat ecosystems, which is consistent with the standard formulation of non-equilibrium thermodynamics. This expression was then compared to five published expressions (4.32, 4.33, 4.34, 4.35, 4.39). Our analysis shows these expressions have major drawbacks. First of all, the contributions from abiotic resource conversion and the environmental reservoirs are neglected in the EP rate. But even accepting such idealizations, they remain problematic, as they are not properly embedded in the standard formulation. Ad hoc expressions are used for the thermodynamic forces and some do not even include these forces at all. Therefore, we conclude that these former propositions cannot always be interpreted as the EP, but comprise other quantities.

## Applications of the entropy production in Lotka-Volterra chemostat ecosystems

We have now an expression for the total and metabolic EP, as well as a set of models. Let us give an outlook for the applications we will encounter in the next chapters. In chapter 6 we will study one favorite LV chemostat system: the resource-consumer-omnivore (RCO). The resource-consumer-predator

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<sup>11</sup>Technically speaking, this EP does not behave as a mathematical Lyapunov function. See glossary or sections 5.7 and 5.8.

(RCP) and the resource-consumer (RC) systems are simplifications that are studied in chapters 7, 8 and 9.

Chapter 3 already spoke of the EP as a candidate goal function: Do ecosystems develop towards an ecosystem metabolism rate at maximum EP? Furthermore, section 4.4.3 also discussed a maximum EP principle. Apparently there is some activity in theoretical ecology that looks for an ecological EP principle [6, 81, 86, 101, 102, 178, 191, 199]. This brings us into contact with a much broader field of research in science: the *maximum entropy production* (MaxEP) concept, which is also studied in a lot of other physical, biological or climatological systems [110, 148]. There is a lot of confusion in the literature concerning the status of MaxEP. The MaxEP ideas in chapter 3 and below eq. (4.39) indicate that there might be different, unrelated MaxEP's. We will see in the next chapter that the situation is quite complicated, as there are basically quite some number of different MaxEP's that are studied in the scientific literature. The only way to deal with them in a systematic way is by constructing a classification in order to disentangle the knots. The major criticism on the MaxEP hypotheses comes in chapter 6. This is where the *RCO ecosystem* comes into play, as it will become a general counterexample (at least at the theoretical level) of the different studied MaxEP hypotheses.

The EP is only one proposal for an ecological *goal function*. There are many other proposals, that will be studied in chapter 7. As the RCO model is a bit too complex, we will look at a simplification, the *RCP ecosystem*, to test those other goal function proposals.

The *goal function* hypothesis in ecology is related with *MaxEP* in physics. But there is another, older discussion that relates ecosystems with some 'dead' physical systems far from thermodynamic equilibrium: the notion of *dissipative structures* [134, 135]. Both the MaxEP hypotheses and the concept of dissipative structures are studied extensively in fluid physics. Chapters 8 and 9 will use the *RC ecosystem* to present an intriguing analogy with dissipative structures in laminar convective fluid systems.

## Chapter 5

# Classification of entropy production principles and hypotheses

### Abstract<sup>1</sup>

The entropy production (EP) is often studied as the basic quantity in organizational or extremal principles. Especially the literature on the concept of maximum entropy production (MaxEP) is steadily growing. Here, a schematic classification of eleven different EP principles and hypotheses is presented, containing the well known least dissipation (Onsager [146]) and the minimum entropy production (Prigogine [159]) principles, as well as eight MaxEP concepts and one gradient response hypothesis. The latter hypothesis states that the EP should increase when the system is driven further out of equilibrium. This classification involves a systematic discussion of all the quantities, constraints, assumptions, applications and ranges of validity for all EP principles/hypotheses. The MaxEP hypothesis in the non-linear response regime are mostly relevant for ecosystems. Therefore, we they will be discussed in more detailed, containing a review of the literature.

### 5.1 MaxEP or MinEP?

It is often claimed [110, 174, 191] that a non-equilibrium system (not necessarily in the steady state) relaxes to thermodynamic equilibrium 'as fast as possible', that it 'follows the most efficient route' to increase its entropy [208] or that it 'selects the path' with highest EP [86]. The idea behind this claim is that a non-equilibrium system is initially in a small region in phase space with low entropy, and has the highest probability to evolve in the next time step to the largest region, with highest entropy. This would result in a maximum of the entropy production (MaxEP). A contradicting argument says that when a system evolves towards the steady state, it will first try to equilibrate those internal parts which are furthest away from equilibrium, because these parts

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<sup>1</sup>This chapter is an extension and refinement of the work in [220]. We also refer to [217] and [221].

have the strongest thermodynamic forces and are therefore the fastest to be attracted to states closer to equilibrium. After a while, the system has used up these strongest forces, and only the weaker forces (which are coming from the externally applied forces) are left for degradation. This results in an initially high EP, but this EP decreases towards a minimum in the final steady state (MinEP).

Both lines of reasoning, one resulting in a MaxEP and the other in a MinEP principle, are quite vague. What is meant by 'selecting a path' or 'an efficient route'? It is difficult to see whether the MaxEP and MinEP really contradict each other. As for the first argument, it is fallacious because the system might not allow evolutions with sudden jumps towards a maximum entropy state. The low entropy and high entropy phase space regions can be highly separated and the microscopic dynamics is constrained to obey some (conservation) laws. Macroscopically, this results in a finite, non-zero relaxation time. Furthermore, the assumptions are not clear: The MaxEP statement highly depends on our way of describing the system (the probability distribution on phase space, the use of deterministic or stochastic microscopic dynamics,...). As for the MinEP argument, under some restrictions (e.g. that the system is in the linear response regime) the MinEP is a valid principle (see discussion in [218]).

The above MinEP and MaxEP arguments were attempts to find a general extremal principle (see Glossary) to understand the behavior of systems. For systems far from thermodynamic equilibrium, such a principle is not known to exist. Nevertheless, in the literature of the last few decades, there is an increase of studies proposing a MaxEP concept. It is intuitively not far fetched to look at the EP, because non-equilibrium systems depend not only on the thermodynamics, but also on the kinetics (dynamics), and the EP, as a bilinear form of forces (thermodynamics) and fluxes (kinetics), is a natural and elegant candidate. The relevant questions are 'What is the central object in the extremal principle?' and 'Can we delineate regions where some principles do apply?'

## 5.2 Why a classification?

The entropy production is used more and more to study physical systems, from simple electrical networks to complex chemical reaction systems, fluid systems or even ecological and climate systems (reviews in [86, 110, 148]). However, there is a possibility for confusion on EP principles. This is not a coincidence, because both MinEP *and* MaxEP apply in the linear response regime [218]. One sometimes uses different words with the same meaning or the same word with different meanings. This is quite often the case for MaxEP. 'Maximum' means 'higher than the rest', but what is the 'rest'? Our crucial statement which we will back up in this chapter, is that there is not one MaxEP, but there are different MaxEP's circling around in the literature, and the differences are not always clearly distinguished. Furthermore, some of those MaxEP's are allowed to be called 'principles', but others are for the moment better termed 'hypotheses' because they are not yet generally accepted as principles.

In this chapter, we will first set up a schematic classification of the different EP principles and hypotheses that are studied in the literature. By an extensive research through numerous scientific studies on EP as an extremal quantity, this leads us to conclude that there are no less than eleven(!) different EP

principles/hypotheses studied: one microscopic and ten macroscopic (see fig. 5.1), which we have named: Least Dissipation, Ziegler's MaxEP, MinEP, Linear Response MaxEP, Non-Variational MaxEP, Partial Steady State MaxEP, Total Steady State MaxEP, Non-linear Lyapunov EP, Non-linear non-Lyapunov MaxEP and Gradient Response. Even more remarkably: Not a single study was found where at least some differences were emphasized. As the macroscopic hypotheses far from equilibrium are the most relevant for ecology, they will be described in more detail.

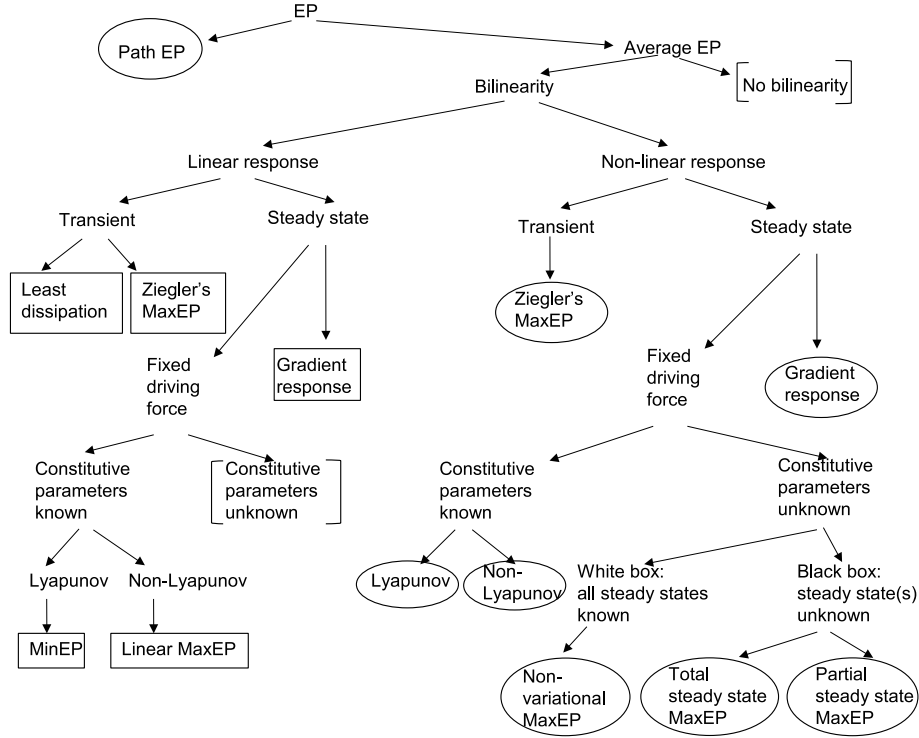


Figure 5.1: The classification of EP principles (in the rectangles) and hypotheses (in the ellipses) that have at least one reference in the literature. The brackets are possible hypotheses which were not (yet) explicitly encountered in the literature.

### 5.3 The classification

Figure 5.1 shows the complete classification of EP principles and hypotheses. The ellipses mean that the hypothesis is generally not correct, whereas the rectangles deserve the name 'principles', because they can be 'proven correct in a non-trivial way' (e.g. by using statistical mechanics arguments).

A first distinction has to be made between microscopic 'path EP' and macroscopic 'average EP'. E.g. Županović and Dewar (private communication) use statistical mechanics arguments to formulate a MaxEP principle for the path EP. Consider a probability measure on path space, the space of all trajectories

in phase space. Each path has at every time a specific EP, called the microscopic EP. The claim is that the microscopic path with highest EP has the highest probability. As we are primarily interested in the macroscopic average EP in ecosystems, we will refer to [217] and [218] for the microscopic approach. It suffices to comment that this microscopic EP hypothesis is not generally valid.

As the name suggests, the macroscopic, average EP hypotheses are only true when looking at averages, i.e. fluctuations can deviate from the average EP behavior [218]. At the macroscopic level, we first have to look for an interesting property: Can the EP be written as a bilinear form of thermodynamic forces and fluxes? As Essex [58] showed, this bilinearity (at least in a 'local' fashion) is not always true for electromagnetic heat radiation. In this chapter, we will restrict to bilinear principles<sup>2</sup>.

To proceed for those bilinear systems, we have to make the distinction between hypotheses in the linear response (LR) and the non-linear response (NLR) regimes. The *linear response* regime [146, 147] is defined to be the regime of forces  $X(C)$  and fluxes  $F(C)$  (with  $C$  the basic macroscopic variables) where the constitutive equations  $F(X)$  are linear (in a sufficient level of approximation):

$$F_\alpha(C) \approx \sum_{\beta} L_{\alpha\beta} X_\beta, \quad (5.1)$$

with  $\alpha$  and  $\beta$  indexing the independent processes (e.g. chemical reactions) and

$$L_{\alpha\beta} = L_{\beta\alpha} = \lim_{X \rightarrow 0} \frac{\partial F_\alpha}{\partial X_\beta}(C = C^{eq}) \quad (5.2)$$

the constant linear response matrix.

Due to these properties, the origin of the principles in the LR regime is much better understood than the NLR hypotheses. In most cases the LR principles are valid. They can be derived (or 'proven correct in a non-trivial way') from both a macroscopic thermodynamics and a microscopic statistical mechanics approach. The four non-trivial principles (least dissipation, Ziegler's MaxEP, MinEP and linear response MaxEP) are understood to follow from fluctuation and large deviations theory [218]. The latter work also made it possible to explain why these principles are invalid for the few counterexamples. We will not discuss the linear response EP principles and the relation between EP and fluctuations, because it would become too technical, and it is not (yet) relevant for our ecological studies.

To avoid confusion, let us point at the fact that linear response is a thermodynamic criterium, relating forces with fluxes. It should not be confused with *linear dynamics*, whereby the approximation

$$F_\alpha(C) \approx \sum_i j_{\alpha,i} C_i \quad (5.3)$$

is sufficient (the  $j$ 's are constant coefficients). The distinction between linear dynamics (LD) and non-linear dynamics (NLD) has nothing to do with thermodynamics, but with dynamics (or kinetics). It is a property of the dynamical

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<sup>2</sup>For non-bilinear systems, no EP hypotheses were found, except one minimum EP principle by Essex [58], for an isothermal black body planet. This MinEP principle is basically the 'non-bilinear' counterpart of the 'bilinear' MinEP studied by Prigogine and co-workers [88]. It shows that the steady state is given by minimizing the EP. The only difference with the 'bilinear' MinEP is that Essex did not minimize the total EP of the total model universe, but only EP associated with the planetary absorption and emission.

equations. We can also make a distinction in NLD systems between systems with a single steady state (or (quasi) periodic) solution or with multiple steady state solutions (or other more complex attractor sets). The first ones will be called 'weakly non-linear systems', the second ones will be termed 'strongly non-linear'. Especially the strongly non-linear systems with multiple steady states will be relevant in later sections and chapters.

Having made the LR-NLR distinction, we move to the third distinction. Some hypotheses are used to find the (constitutive or dynamical) equations of motion, rather than the (steady) state of a system. The so called 'transient' principles are basically Lagrangian (or Hamiltonian) principles, where the variation of a functional (a function on the space of functions of the macroscopic variables  $C(t)$ ), called the Lagrangian  $\mathcal{L}(C(t))$ , is performed in order to find the dynamical (written as  $\dot{C}(F(C))$ ) or the constitutive (written as  $F(X)$ ) equations of motion. These equations of motion are valid in both the transient and the steady states. The 'steady state' hypotheses are as the name suggests used to find the steady state(s) of the system. More generally, by taking time averages, they can be used to find attractor (steady, periodic, quasi-periodic or chaotic) states [122, 133]. For simplicity, in this work we will always look at steady states instead of the more general attractor states. Steady states will be denoted with a superscript  $*$ .

Studying the steady states requires knowledge of the externally applied thermodynamic force. Therefore, within these steady state hypotheses one has to make a distinction between systems where the external force is known and fixed and systems that study the behavior of the steady state(s) when the external force is varied. The latter we called the gradient response hypotheses, because they discuss the response of the system when the gradient, or the external driving force, changes. Questions like 'does the EP increase when the system is driven further out of equilibrium?' and 'how sensitive is the EP under changes in the force?' are studied in the gradient response hypotheses.

For the systems where the external driving force is kept fixed, one can make a next distinction, depending on our knowledge of the system. After all, extremal principles are only relevant when a full knowledge of the system (the equations of motion and its solutions) is absent. One now has to ask 'What is the minimum amount of knowledge required to find the true (physically selected) steady state?' In all hypotheses which are classified under the 'fixed driving force' condition, a full knowledge of the dynamical equations of motion  $\dot{C}(F(C))$  is not necessary. But for some hypotheses a full knowledge of the constitutive equations of motion  $F(X)$  is required, because these expressions contain information to construct a generalized potential  $\mathbf{L}(C)$ , i.e. a function on the space of macroscopic variables  $C$  which is extremal in the steady state  $C^*$ . In order to find the steady state, the potential is constrained and knowledge of these constraints is necessary. Depending on the type of constraints used in these variational principles, one can make a distinction between Lyapunov and non-Lyapunov principles. A Lyapunov principle has a generalized potential, the Lyapunov function, with  $\mathbf{L}(C^*)$  maximum (or minimum) and  $\frac{dL}{dt} \geq 0$  (or  $\leq 0$ ). Therefore, the Lyapunov principle contains some non-trivial information about the evolution along transient states.

Some EP hypotheses at fixed external driving force are also applied to systems where there is no complete knowledge of the constitutive equations (e.g. some parameters  $\kappa$  are a priori unknown). In this case, two kinds of hypotheses

are in use. The first one requires a knowledge of the values of all the steady states, plus the expression for the EP in those steady states. The hypothesis can be formulated as "the selected steady state is the one with a higher EP than the other steady states". This is the so called 'white box' principle, because we can look into the system and know its possible states. It is a principle that selects the true steady state (e.g. the most asymptotically stable) amongst the discrete set of all possible steady states. This is not a variational principle, because there is no quantity (action or generalized potential) depending on continuous variables which are varied in order to find the extremum.

The second hypothesis involves a 'black box' approach, where knowledge of the steady states is absent and the dynamical and constitutive equations are partially known. One only has the knowledge of some elements in the constitutive equations, the external driving force and the steady state conditions (equations like e.g.  $\sum_{\alpha} F_{\alpha} = 0$ ). A variational principle is used whereby a quantity  $\hat{\mathbf{L}}(\kappa) = \hat{\mathbf{L}}(C^*(\kappa), \kappa)$  is varied with respect to the a priori unknown parameters  $\kappa$ . These parameters are typically appearing in the constitutive equations. This 'black box' approach is used especially in far-from-equilibrium systems with highly complex dynamics. In these highly complex systems, there can be a big difference in timescales of different variables and processes. For example in ecosystems, one has the very short timescale for chemical reactions, a short timescale corresponding with e.g. behavior of individuals, a longer timescale for population dynamics and a very long timescale for evolution and natural selection. The parameters  $\kappa$  are typically treated as 'effective' or 'dynamical' parameters, i.e. they can depend on variables with timescales much longer than the ordinary variables  $C(t)$ . The steady state  $C^*(\kappa)$  becomes in fact a pseudo steady state, because the  $\kappa$  can slowly change. Basically  $\hat{\mathbf{L}}(\kappa)$  is a long timescale Lyapunov function on 'dynamical parameter' space. For the EP applications in the literature, this 'black box' principle (hypothesis) comes in two kinds: one sometimes uses the total EP and sometimes a partial EP, corresponding with a specific important but highly complex process. Both total and partial EP are under steady state conditions.

This gives the overview of the classification. We will now give some further discussion and literature review of the macroscopic EP hypotheses in the non-linear response regime. These are especially interesting for strongly non-linear systems far from equilibrium, such as fluid, climate and ecosystems. All these non-linear EP ideas are still at the level of hypotheses, i.e. they have not (yet) very strong experimental or theoretical underpinning. The reader interested in the linear response principles is referred to [220].

## 5.4 Non-Variational MaxEP

When the dynamics  $\dot{C}(F(C))$  is highly non-linear, the system might have different steady states  $X_{\alpha}^{\gamma}(C^{\gamma})$ ,  $F_{\alpha}^{\gamma}(C^{\gamma})$  with  $\gamma$  counting the different steady states. Suppose we know these steady states, but we do not know which one is physically selected by the system. One has to make the notion 'selected' mathematically more precise. The selected state might be e.g. the most stable one<sup>3</sup>. Further-

<sup>3</sup>Another possibility is that the state with the largest (relative) size of its basin of attraction is most likely chosen. The basin of attraction is the set of points in state space such that initial conditions chosen in this set will evolve under the dynamics towards the attractor state (e.g.

more, one has different notions of stability [133], such as asymptotic stability. Having chosen a precise notion of 'selected', the non-variational MaxEP hypothesis claims that the selected steady state (written with upperindex  $\gamma = *$ ) is the one with highest EP:

$$\sigma^*(X^*, F^*) \geq \sigma^\gamma(X^\gamma, F^\gamma), \quad \forall \gamma. \quad (5.4)$$

An important remark is that this MaxEP hypothesis is not a variational principle, because there is no Lagrangian or generalized potential and no variation with respect to continuous variables such as fluxes. It is rather a selection principle of a discrete number of steady states. Furthermore, the non-variational MaxEP does not claim that the EP always increases in time if the system evolves towards the 'selected' steady state.

This MaxEP hypothesis is also related to the notion of dissipative systems with dissipative structures (see chapter 8. If one drives the system out of equilibrium, at certain critical points of the driving force, bifurcations to other stable states are possible. Then a patterned or ordered structure might arise. A famous example is the Rayleigh-Bénard system [162] which we will encounter in chapter 9. Ordered convection cells (the dissipative structures) appear in a fluid layer which is sufficiently heated from below. The claim is that these ordered dissipative structures (if they exist) always have a higher EP than the so called 'thermodynamic branch' states without the structures, i.e. the states which do not show a pattern. Especially Schneider et al. [179] describe the increase in EP when the Bénard fluid system moves to the stable convection state.

This MaxEP hypothesis has some other experimental verifications from a number of studies, especially in field of fluid dynamics. Apart from the Bénard system, Shimokawa et al. [149, 184], based on work by e.g. Malkus [107], studied turbulent and (oceanic) fluid systems, and they discovered that the MaxEP state is most stable against perturbations. Rennó [164] suggested that the most stable state in a radiative-convective atmosphere model with two stable states has the highest EP. Also in the Brusselator chemical reaction system, non-variational MaxEP was observed with numerical simulations (see e.g. Sawada<sup>4</sup> [175].) Christen [36] mentions applications for nonlinear electrical systems (non-linear conductors such as gas dischargers or semiconductors). These non-linear systems often exhibit multistability, and MaxEP would select the steady state with highest EP.

The above mentioned studies were applied to systems with fixed boundaries. One also observed a possible non-variational MaxEP principle in non-steady systems with growing boundaries, like the morphology of crystal growth [111] or growing random surface patterns [175, 174]. For these systems one might have a time dependent EP as  $\sigma \propto t^\alpha$ . The most stabilized mode of growth is argued to be the one with highest exponent  $\alpha$ . Like the steady state selection, this is a 'mode of growth' selection principle. We will not deal with the latter in this thesis, although they might potentially be relevant for biological growing systems.

A critical remark to the non-variational MaxEP hypothesis is that there is no general proof, and some studies even showed possible counterexamples.

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the steady state). This approach is useful when knowledge of the initial conditions are missing.

<sup>4</sup>Sawada called it confusingly a variational principle, although there was not a clear notion of a variational quantity presented.

As mentioned above, the non-variational principle deals with multiple steady states, and the external driving force (e.g. the temperature gradient) is an important parameter. When this parameter increases, bifurcations towards new patterns and dissipative structures might occur. Most of the above mentioned studies were restricted to the dissipative structures after the first bifurcation (e.g. the transition from the conduction to the convection state in the Rayleigh-Bénard system). However, when the system is pushed further out of equilibrium, new bifurcations might arise, resulting into new states or patterns (e.g. wavy convection, turbulence,...). And as is shown by numerical simulations [31, 38, 130, 131, 132], the total heat transport and EP of these new states might be lower. Nicolis [132] also gave a counterexample of the non-variational MaxEP hypothesis for chemical reactions. In later chapters (6, 7, 8), we will see some ecosystem models as counterexamples to the non-variational MaxEP hypothesis. Contrary to the numerical simulations in [31, 38, 130, 131, 132] (which were criticized in [110] precisely because of numerical problems), our models will be analytically solvable (and the criticism of [110] does not apply to our studies). Since non-variational MaxEP is not always valid, the search is for criteria and restrictions on the dynamics for the situations where it is valid.

A second critical remark is that the non-variational MaxEP hypothesis is often confused with other principles. In e.g. [208], the non-variational MaxEP is misleadingly related with a variational principle, the least dissipation, without stressing its differences. Also in [50] the author mentions a proof for the linear response MaxEP and discusses (without mentioning the differences) a non-variational MaxEP (the Rayleigh-Bénard system) and a partial steady state MaxEP (the atmosphere climate system by [151], as we will see in the next section). Furthermore, in e.g. [149] and in the reviews e.g. [148] and [110], both the partial steady state and non-variational hypotheses were discussed without stressing their differences.

## 5.5 Partial Steady State MaxEP

In chapter 3, we encountered a MaxEP hypothesis: there was an unknown effective parameter, the ecosystem metabolic rate  $\kappa_{EM}^*$ , and the hypothesis was that the associated EP was maximum for a specific value of this parameter. This is an example of the interesting partial steady state MaxEP hypothesis. We will give a short overview of the literature below.

The basic formulation of this variational MaxEP principle is the following. Suppose that all the constitutive equations  $F(X)$  are known, except for one  $F_\kappa(X, \kappa)$ , because e.g. some 'effective parameter'  $\kappa$  is unknown.<sup>5</sup> Furthermore, suppose that the system is known to be in a steady state, without knowing the values of  $C^*$ ,  $F^*$  and  $X^*$ . The objective is to find  $F_\kappa^*(X^*)$ . As  $F_\kappa^*$  is a function of the unknown  $\kappa^*$ , it is equivalent with finding the correct value  $\kappa^*$  which maximizes some variational quantity  $\mathbf{L}(F(\kappa))$ . The partial steady state MaxEP is a variational principle

$$\mathbf{L}(F(\kappa)) = X_\kappa F_\kappa + \sum_\nu \lambda_\nu \left( \sum_\alpha \beta_{\mu\alpha} X_\alpha - X_\nu^0 \right)$$

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<sup>5</sup>The principle can be generalized to more unknown constitutive equations, as well as unknown  $X_\kappa$ , but we will not go into this subtle issue because all examples discussed in this thesis will have only one unknown.

$$+ \sum_{\zeta} \lambda_{\zeta} (\sum_{\alpha} \beta_{\zeta\alpha} F_{\alpha} - F_{\zeta}) + \sum'_{\alpha} \lambda_{\alpha} (F_{\alpha} - F_{\alpha}(X)). \quad (5.5)$$

The first term indicates that not the total EP, but only the partial EP term corresponding with the unknown  $F_{\kappa}$  is considered as the basic quantity in this variational principle. The sums with the Lagrange multipliers  $\lambda_{\nu}$  and  $\lambda_{\zeta}$  are constraints included to look for the steady state.  $X_{\nu}^0$  is a constant externally applied force, and thermodynamic consistency requires some relation between the forces (e.g. Kirchoff's loop law in electrical circuits or Hess's law in chemical reaction systems are constraining the fluxes). The constraints with multipliers  $\lambda_{\zeta}$  are the steady state conditions ( $\dot{C} = \sum F = 0$ ). This means that the steady state conditions (not the states themselves) should be known when applying this principle. The final sum are the constraints for the constitutive equations  $F = F(X)$ . Notice that we have written a prime on the summation, because the unknown  $\kappa$ -th term is absent, i.e. knowledge of  $F_{\kappa} = F_{\kappa}(X)$ , including all quantities (such as  $\kappa$ ), is absent.

Let us give a simple example. Consider two electrical resistors (at the same temperature) in series and coupled with a constant external voltage  $U^0 = TX^0$ . Let us take the temperature  $T = 1$  for simplicity. Suppose the first resistor is in the linear response regime, with its value  $R_1$  fixed and known. The second resistor is now considered as a 'black box', i.e. we do not know its constitutive equation, which might be highly non-linear. The partial EP  $X_2 F_2$  is maximized under the steady state conditions (Kirchoff's laws,  $X_1 + X_2 = X^0$  and  $F_1^* = F_2^*$ ) and Ohm's law ( $X_1 = R_1 F_1$ ) for the first resistance. This gives

$$\begin{aligned} \hat{\mathbf{L}}(F(\kappa^*)) &= X_2^* F_2^* = (X^0 - X_1^*) F_1^* \\ &= (X^0 - R_1 F_1^*) F_1^*. \end{aligned} \quad (5.6)$$

Maximizing with respect to  $F_1^*$  gives  $F_1^* = \frac{X^0}{2R_1}$ . If one would write  $X_2^* = R_2^* F_2^*$ , then the unknown second resistor value (the unknown effective parameter  $\kappa^*$ ) in the steady state equals  $R_2^* = R_1$ . This derivation is completely analogous to the maximum power theorem in electrical systems and control thermodynamics [74, 169], which states that to obtain maximum power from a source with a fixed internal resistor (the first resistor), the resistor of the load (the second resistor) must be made the same as that of the source.

Of course this principle is not true in general: One can simply take a second resistance different from the first one. So why is this principle relevant anyway? It is believed to be valid in (some) systems far from equilibrium, with highly non-linear behavior and with sufficient variables (many degrees of freedom), such that the unknown dynamical parameter  $\kappa^*$  is flexible, and it will (perhaps by self-organizing evolution, trade-offs and negative feedbacks) be most probable (when the number of degrees of freedom is very large) to settle itself at the optimal value. The correct explanation is not known yet, nor is there a non-trivial theoretical model which shows this MaxEP behavior. There are a number of proposals, but there is not yet a proof based on first principles. Let us briefly mention a few.

-Dewar [49, 50] tried to derive the MaxEP from a microscopic, path-information perspective. It states that if one associates a probability to every microscopic path, then perhaps this probability measure in path space results (by maximizing the path-information entropy) into a most likely macroscopic trajectory

with MaxEP. It is suggested that it only works for systems with sufficient degrees of freedom, such that a kind of law of large numbers can be applied. These kind of arguments are sometimes believed to be an underlying explanation for MaxEP (see also [86]). Dewar's reasoning was shown to be invalid (or at least incomplete) in [217], and its appendix discussed the relation between the partial steady state MaxEP and the maximum entropy principle.

- Ozawa et al. [148] discuss a feedback mechanism. Roughly speaking, it is based on a trade-off: If the steady state flux  $F_{\kappa}^*$  increases, then the conjugate force  $X_{\kappa}^*$ , i.e. the driving force inside the system, decreases and vice versa (this can easily be seen in the above electrical circuit example). In other words, at one end of the  $\kappa^*$ -spectrum the system is slow (low  $F_{\kappa}^*$ ) but too far from internal equilibrium, as measured by the 'internal frustration' of the force  $X_{\kappa}^*$ . At the other end of the spectrum the 'internal frustration' is low, but the system needs to sustain a flux which is too high. For a specific value of  $\kappa^*$  in between those two end-members, the product  $X_{\kappa}^* F_{\kappa}^*$  is maximal.

- Paltridge [152] uses an argument based on fluctuations. Some fluctuations are damped, other gain energy, moving the system to the MaxEP state.

- Perhaps the system has many steady states, and perhaps most of them are 'clustered' around the MaxEP value. This might increase the probability of selecting a steady state close to MaxEP.

These and other proposals are still quite vague and they need to be studied further in order to find the correct explanation. We will come back to this issue in chapter 10.

From a theoretical point of view, the search for a non-trivial but analytically solvable model showing MaxEP is the major challenge. Also other questions need to be resolved: What if multiple  $\kappa^*$  or  $F_{\kappa}^*$  were unknown? Which combination of EP's should be used in that case? What about differences in time and spatial scales? How much variables or degrees of freedom are needed? How non-linear should the system be? What are the basic assumptions? Can it be derived from first principles, or is it a new law for some systems? What about disturbances away from the MaxEP state? Is there a relaxation process towards MaxEP (with Lyapunov-like behavior  $d(X_{\kappa} F_{\kappa})/dt \geq 0$ )? Can one find a non-trivial model showing partial steady state MaxEP? Are there necessary underlying constraints in order that this MaxEP is valid?

Apart from attempts for a theoretical underpinning, there is also an increasing amount of experimental verification, and the hypothesis is also used as a modeling technique. So let's have a brief overview of the literature concerned with this hypothesis. We already mentioned the climate studies in section 3.6, and the relation with ecological systems. But perhaps also in older ecological studies this MaxEP hypothesis appeared. Starting with the above mentioned maximum power theorem [74], Lotka, Odum and others (see e.g. [70, 144]) extended this maximum power theorem to ecosystems. However, as these works are quite difficult to interpret in a MaxEP way, it is yet unclear whether this extension by Lotka et al. to ecosystems is really the partial steady state MaxEP hypothesis. Also Cai et al. [27] performed some empirical investigation on the maximum power hypothesis, but as they did not specify e.g. the thermodynamic forces, this experimental study might be unrelated with the MaxEP hypothesis. In contrast, chapter 3 gave a much clearer perspective, which is new in the ecological literature. There are (very!) rough experimental indications that this MaxEP might work for specific ecosystems like sediment ecosystems

at the bottom of the sea [219]. Further research is required to make this MaxEP convincing.

Also (sub)cellular biological systems are studied in the light of this MaxEP hypothesis. Juretic et al. applied MaxEP to biochemical reactions, especially photosynthesis [82] and ATP synthesis [51]. The chemical reaction system of ATP synthase consists of compartments (the different molecular states) with particle fluxes between them. A parameter  $\kappa$  and the flux  $F(\kappa)$  between the compartments O:ATP and O:P.ADP are unknown. The most likely values for this parameter and flux were derived by maximizing the corresponding EP (not the total EP of all reactions), knowing that the system is in the steady state. The functional description of this ATP synthase chemical reaction system (the distinction between compartments and the non-linear interactions between some of them) is very analogous to our chemotrophic ecosystem studied in chapter 3.

Apart from trying to explain MaxEP, another approach is to accept it and use it as a modeling technique for self-organizing climates and Gaia-models [195]. But this approach was criticized by [1] who showed that the daisyworld Gaia-model did not evolve to the MaxEP state. On the other hand, Kleidon [85] argued that there is a correspondence between MaxEP and Gaia: The biosphere evolves towards the MaxEP state and since this state is in homeostasis due to negative feedbacks, the biosphere creates a homeostatic state 'by and for itself', which is the formulation of the Gaia hypothesis. The discussion pro or contra Gaia-MaxEP remains unsettled.

Chapter 6 contains a general counterexample of all non-linear MaxEP hypothesis, also the partial steady state MaxEP. However, more will be said on this issue in chapter 10, where we will make a distinction between the macroscopic and the megascopic scale. The counterexample in chapter 6 only applies to the macroscopic level, leaving open the possibility for MaxEP at the megascopic level.

## 5.6 Total Steady State MaxEP

The total steady state MaxEP was also encountered in chapter 3, and it is similar to the partial steady state MaxEP, except that one now uses the total steady state EP  $\sigma^*(X^*, F^*)$  (note that this is also used in the non-variational MaxEP) instead of the partial steady state EP  $X_\kappa^* F_\kappa^*$ . When there is only one external driving force  $X^0$  and a conjugate flux  $F$ , the total steady state EP looks like  $\sigma = X^0 F^*$ . Simply maximizing this quantity with respect to  $F^*$  is meaningless because it results in an infinity. The reason why the steady state MaxEP does not apply to the total EP is that there is no trade-off. For a partial EP, one could have a non-fixed  $X_\kappa$  which might decrease when its conjugate  $F_\kappa$  increases. Hence, due to this trade-off one avoids meaningless infinities.

Another possibility is performing an extremization with respect to unknown effective parameters  $\kappa^*$ . The idea is that the system can change these parameters such that e.g. its uptake of free energy from the environment is increased. This free energy is then dissipated by the system, and therefore the total dissipation increases.

Let us go back to the electrical circuit example with two resistances, the second being a 'black box'. The total steady state EP would be  $\sigma^* = (X^0)^2 / (R_1 + R_2^*)$ , and this becomes maximal when  $R_2^* \rightarrow 0$ . As a physical example, Kleidon

[85] looked at a planetary system with a variable albedo as effective parameter. It was used in e.g. in planetary climate and ecosystems, as discussed in e.g. [85]. There is a constant inflow of solar radiation at the earth, but part of this low entropy radiation is reflected. However, it is claimed that biological systems evolve such as to capture more efficiently this incoming radiation, turning it into high entropy heat radiation. So the ecosystem lowers its internal parameter  $\kappa^*$ , the planetary albedo, and the highest EP is reached when the albedo is zero. The earth with zero albedo becomes a black body and as is shown in [172], the black-body radiation is indeed in the MaxEP regime. Due to the fact that the earth albedo is not (yet) zero, this MaxEP state is not (yet) reached. We will discuss a phototrophic ecosystem model with variable albedo in chapter 8.

The total steady state MaxEP was also used by Christen [36] for the Steenbeck principle for electric arcs in highly nonlinear electric systems: "The steady state of a real gas discharge minimizes its energy conversion (i.e. heat power) and thus its voltage." It is related to the above electrical circuit example: Suppose that the second resistor is an electric arc (a plasma of a gas discharge) with 'effective' resistance  $R_2(F)$  that depends on the current  $F$  as well as on some other variables (or effective parameters)  $\kappa$ , e.g. the temperature inside the arc plasma. It is possible that the system will settle in the state with values  $\kappa^*$ , such that the total EP is maximal (as compared to the EP values for other possible values of  $\kappa^*$ ) for constant external voltage  $X^0 = F(R_1 + R_2)$ . Writing  $R_1\sigma^* = (X^0)^2 - X^0X_2^*$ , with  $X_2^* = F^*R_2^*$  the voltage over the electric arc, we see that MaxEP means that the steady state of a gas discharge system also minimizes the voltage  $X_2^*$  with respect to  $\kappa^*$ , something which has experimental verification (see [36] for more references).

As for the theoretical underpinning, the appendix of [50] contains a possible explanation, but its validity is still under discussion, as was demonstrated in [217].

## 5.7 Non-linear Lyapunov EP

In the linear response regime, there is a famous MinEP principle [88]. The EP behaves as a Lyapunov function. Lyapunov functions compare transient states with steady state(s). Near the steady state, the EP monotonously decreases towards a minimum in the steady state. MinEP is no longer true in the non-linear regime, but a priori in some regimes far from equilibrium, Lyapunov MinEP or MaxEP could be possible. However, no clear examples of non-linear Lyapunov EP are known. We mention the principle here for completeness sake, and also because it is related with the ecological goal function literature, as we will see in chapter 7.

We have also mentioned the possibility that the partial steady state MaxEP might be a Lyapunov principle. Basically it comes down to the timescales involved. Some variables  $C_i(t)$  might change rather fast (timescale  $t$ ) and settle in a steady state  $C_i^*(\kappa^*)$ , depending on the parameters  $\kappa^*$ . But these parameters might not be constant<sup>6</sup>, but they might change very slowly, at a very long timescale  $\tau$ . This is what happens in ecosystems, where there is a fast ecosystem dynamics (with fast variables  $C(t)$ ) and a very slow evolutionary dynamics (with slow variables  $\kappa^*(\tau)$ ). Hence, there can be a Lyapunov function on the space

<sup>6</sup>The superscript \* now refers to the (quasi) steady state for timescale  $t$ .

spanned by the  $C$ 's or the  $\kappa^*$ 's. The latter Lyapunov behavior was mentioned in the discussion on the partial steady state MaxEP.

## 5.8 Non-linear Non-Lyapunov MaxEP

In chapter 4, after eq. (4.39), a MaxEP idea was discussed (which was incorrectly called 'MinEP' in [81]). The mathematical structure of this hypothesis (as used in e.g. [81]) is equivalent with the Linear Response MaxEP, which is also a non-Lyapunov principle [220]. The EP (as a function of the  $C$ 's) is varied under a constraint (e.g. constancy of biomass in [81]). The maximum of the EP with respect to this constraint gives the steady state of the dynamics (e.g. generalized Lotka-Volterra dynamics in [81]). The constraint is often only a mathematical 'trick', because e.g. in generalized LV dynamics there is no biomass conservation law. As this MaxEP does not claim that  $d\sigma/dt \geq 0$ , the EP does not behave as a Lyapunov function on the state space spanned by the  $C$ . Furthermore, in [81], very restrictive assumptions were required (see chapter 4) to obtain the correct thermodynamic EP expression as a quadratic function. Therefore, we believe that this principle is of less value and without much experimental relevance.

## 5.9 Gradient Response

The above hypotheses were variational or non-variational principles with a fixed external driving force (also called an applied gradient). Schneider and Kay [179] studied the degradation of an applied gradient, resulting in EP. What Schneider and Kay basically did, was looking at the change in EP when the external driving force is increased. They formulated what they have called a 'restated second law of thermodynamics'.

"The thermodynamic principle which governs the behavior of systems is that, as they are moved away from equilibrium, they will utilize all avenues available to counter the applied gradients. As the applied gradients increase, so does the system's ability to oppose further movement from equilibrium."

We have called this hypothesis the maximum gradient response. It needs some further specification, because it is still quite vague.

We can give at least three different interpretations, from the most general (weak) to the most restrictive (strong). These interpretations are formulated as: For the physically selected steady state

- the EP is positive.
- the EP is increasing as the gradient increases.
- the EP is increasing and it is a steeper function compared with the EP of the unselected steady states.

Again, as in the non-variational MaxEP, the notion of the 'selected' state can be interpreted in different ways. The possibility that we will choose is the 'most asymptotically (linear) stable' state. The first of the above statements is nothing but the second law. The latter two statements are a weak and a strong extension.

Metaphorically speaking, one can think of a mountain river. The steepness of the mountain would correspond with the gradient (external driving force) and

the flow of the river is the thermodynamic flux (e.g. a chemical reaction rate). The product of steepness and flow resembles the EP. The gradient response now compares different mountain rivers: The steepest river should have the strongest flow.

The weak gradient response hypothesis is also related to the work by [208], where the behavior under quasi-stationarity conditions was studied: When the external reservoirs are very large but finite (as is the case in real systems), the intensive quantities (e.g. the temperature) are no longer constants but they become slowly variable. The environmental reservoirs are very slowly relaxing towards global equilibrium or in other words, the gradient slowly decreases. It was claimed by Woo that  $\frac{d\sigma^*}{d\tau} \leq 0$ , with the  $*$  denoting the quasi steady state value and  $\tau$  the time corresponding with the long time scale of this slow relaxation process.

The gradient response hypothesis is true in the linear response regime, because there is only one steady state and the EP is always quadratic. But as we will demonstrate in a later chapter with a resource-consumer-omnivore ecosystem which is far from equilibrium, the selected steady state EP is not always increasing.

## Chapter 6

# Testing entropy production hypotheses in ecosystems

### Abstract

Using the expression for the entropy production (EP) in a chemotrophic ecosystem with one resource type, one consumer species and one omnivore species, we can test different EP hypotheses. In particular, we study whether the most stable steady state is the one with the highest EP (the 'non-variational' MaxEP hypothesis), whether the EP of the ecosystem metabolism settles into a maximum (the 'partial steady state' MaxEP hypothesis), whether the EP increases under ecosystem evolution or population dynamics (the 'total steady state' and the 'Lyapunov' MaxEP hypotheses), and whether the EP increases if the system is driven further out of equilibrium (the gradient response EP hypothesis). It is shown that there are parameter values (that are a priori not unphysical) such that none of these hypotheses are valid. We conclude with a critical discussion about possible relations between the trio 'ecosystem EP', 'ecosystem stability' and 'biodiversity'.

### 6.1 Introduction

In the previous chapter we demonstrated that there are different MaxEP hypotheses. Especially the hypotheses in the non-linear response regime are on shaky ground. If proofs are absent, can one find counterexamples?

Ecosystems operate far from equilibrium, outside the non-linear response regime. Looking at the chemotrophic ecosystems (chapters 3 and 4), it is easy to see that linearity is absent: Both the dynamics  $\dot{C} = F(C)$  and the constitutive equations  $F(X)$  are non-linear. Therefore, ecosystems can be counterexamples to MaxEP hypotheses. Here we will see that there is especially one elegant model, the resource-consumer-omnivore (RCO) chemostat ecosystem, because this one model will serve as a theoretical counterexample to basically all non-linear MaxEP hypotheses.

What makes this RCO ecosystem especially interesting is the existence of a region with multiple stable steady states. That multistability regime is highly intriguing from both an ecological and a thermodynamic perspective. From the ecological point of view, this multistability might result in catastrophic

regime shifts [176]. Small perturbations can have drastic consequences, such as the sudden extinction of a complete population. From a thermodynamic perspective, the behavior of the EP will be interesting and perhaps counter-intuitive. We will clarify this intriguing behavior below.

## 6.2 The resource-consumer-omnivore ecosystem

Let us consider a generalized LV chemostat system as in (4.19-4.21) with one resource at concentration  $C_R$ , a consumer with biomass concentration  $C_C$  and an omnivore with biomass concentration  $C_O$ . The omnivore is a predator that also directly feeds on the resource [73, 128]. We take complete recycling (ratios  $r = 1$ ) and fast waste exchange  $\alpha_W \rightarrow \infty$ . The latter means that  $C_W \approx C_W^0 \equiv K_{eq} C_R^{eq}$  with  $C_R^{eq}$  the chemical equilibrium value for the resource concentration.

The population dynamics now look like:

$$\begin{aligned} \frac{d}{dt} C_R &= \alpha_R(C_R^0 - C_R) - (\kappa_{AC} + g_{CR}C_C + g_{OR}C_O)(C_R - C_R^{eq}) \\ &\quad + d_C C_C + d_O C_O, \end{aligned} \quad (6.1)$$

$$\frac{d}{dt} C_C = q_{CR}g_{CR}(C_R - C_R^{eq})C_C - g_{OC}C_C C_O - d_C C_C, \quad (6.2)$$

$$\frac{d}{dt} C_O = q_{OC}g_{OC}C_C C_O + q_{OR}g_{OR}(C_R - C_R^{eq})C_O - d_O C_O. \quad (6.3)$$

The associated ecosystem metabolism is given by

$$\begin{aligned} F_{EM} &= (\kappa_{AC} + (1 - q_{CR})g_{CR}C_C + (1 - q_{OR})g_{OR}C_O)(C_R - C_R^{eq}) \\ &\quad + (1 - q_{OC})g_{OC}C_C C_O. \end{aligned} \quad (6.4)$$

We can now study the steady states by putting all time derivatives equal to zero. These steady states will be studied in function of the thermodynamic gradient, defined by

$$\Delta \equiv C_R^0 - C_R^{eq}. \quad (6.5)$$

This gradient will serve as a bifurcation parameter. Confirming the results of previous model studies on omnivory [128], linear stability analysis shows that there are at most five stationary states, and four critical bifurcation points:

$$\Delta_{c1} = \frac{\alpha_R + \kappa_{AC}}{\alpha_R} \frac{d_C}{q_{CR}g_{CR}}, \quad (6.6)$$

$$\Delta_{c2} = \frac{A \left[ \left( C_R^{eq} + \frac{d_C}{q_{CR}g_{CR}} \right)^2 - (C_R^{eq})^2 \right] + B \frac{d_C}{q_{CR}g_{CR}}}{\alpha_R q_{OC} g_{OC}}, \quad (6.7)$$

$$\Delta_{c3} = \frac{A(C_R^{eq})^2 + B C_R^{eq} + B^2/(4A)}{\alpha_R q_{OC} g_{OC}}, \quad (6.8)$$

$$\Delta_{c4} = \frac{A \left[ \left( C_R^{eq} + \frac{d_O}{q_{OR}g_{OR}} \right)^2 - (C_R^{eq})^2 \right] + B \frac{d_O}{q_{OR}g_{OR}}}{\alpha_R q_{OC} g_{OC}}, \quad (6.9)$$

with

$$A = g_{OR}g_{CR}(q_{OC}q_{CR} - q_{OR}), \quad (6.10)$$

$$B = -2AC_R^{eq} + (\alpha_R + \kappa_{AC})q_{OC}g_{OC} + d_Cg_{OR}(q_{OR} - q_{OC}) + d_Og_{CR}(1 - q_{OC}q_{CR}), \quad (6.11)$$

$\Delta_{c1}$  and  $\Delta_{c2}$  are transcritical bifurcations, whereas  $\Delta_{c3}$  and  $\Delta_{c4}$  are the limit points of saddle-node (jump) bifurcations. Figure 6.1 plots the resource, consumer and omnivore concentrations.

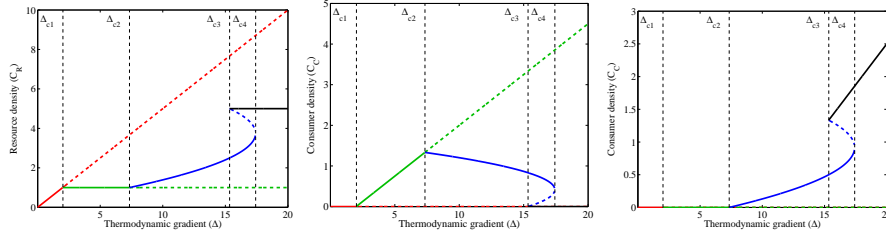


Figure 6.1: Resource-consumer-omnivore food web. Bifurcation plot of the resource concentration  $C_R$  (kmol C m<sup>-3</sup>), consumer biomass density (mol C m<sup>-3</sup>) and omnivore biomass density (mol C m<sup>-3</sup>) at steady state as a function of the thermodynamic gradient  $\Delta$  (kmol C m<sup>-3</sup>). The dashed lines are the unstable states, the solid lines are stable states. The red states are abiotic, green states contain a monoculture of consumers, blue states are consumer-omnivore coexistence and black states are a monoculture of omnivores. The parameter set that was used is:  $\alpha_R = 0.01$  yr<sup>-1</sup>,  $q_{CR} = 1/5$ ,  $d_C = 10$  yr<sup>-1</sup>,  $g_{CR} = 50$  yr<sup>-1</sup> per mol C of resource,  $q_{OC} = 1/5$ ,  $d_O = 10$  yr<sup>-1</sup>,  $g_{OC} = 30000$  yr<sup>-1</sup> per mol C of consumer,  $\kappa_{AC} = 0.01$  yr<sup>-1</sup>,  $C_R^{eq} = 0.01$  mol C m<sup>-3</sup>,  $q_{OR} = 1/5$  and  $g_{OR} = 10$  yr<sup>-1</sup> per mol C of resource. This way, the omnivore's growth is slower when feeding on resource as compared to its preying on the consumer.

The asymptotically (linearly) stable stationary state solutions (for  $A < 0$ ) for the resource concentrations are<sup>1</sup>:

If  $\Delta \leq \Delta_{c1}$ :

$$C_R^* = C_R^{eq} + \frac{\alpha_R \Delta}{\alpha_R + \kappa_{AC}}. \quad (6.12)$$

If  $\Delta_{c1} \leq \Delta \leq \Delta_{c2}$ :

$$C_R^* = C_R^{eq} + \frac{d_C}{q_{CR}g_{CR}}. \quad (6.13)$$

If  $\Delta_{c2} \leq \Delta \leq \Delta_{c4}$ :

$$C_R^* = \frac{-B + \sqrt{B^2 + 4A(\alpha_R q_{OC} g_{OC} \Delta + B C_R^{eq} + A(C_R^{eq})^2)}}{2A}, \quad (6.14)$$

If  $\Delta_{c3} \leq \Delta$

$$C_R^* = C_R^{eq} + \frac{d_O}{q_{OR}g_{OR}}. \quad (6.15)$$

<sup>1</sup>We will not give the explicit expressions for  $C_C^*$  and  $C_O^*$ , because they do not appear in the total steady state EP expression.

Note that if  $\Delta_{c3} \leq \Delta_{c4}$ , the region between these two bifurcation levels has two stable steady states. One state represents a coexistence of consumer and omnivore species, and the other is a monoculture of omnivores whereby the consumer is extinct (see fig. 6.1). This multistability region will become important in the discussions below.

In the steady state, the ecosystem metabolism equals the resource exchange

$$F_{EM}^* = F_R^* = \alpha_R(C_R^0 - C_R^*) \quad (6.16)$$

and the total EP is (see chapter 3)

$$\sigma_{tot}^* = \alpha_R(C_R^0 - C_R^*)R \ln \frac{C_R^0}{C_R^{eq}}, \quad (6.17)$$

As they are given by  $C_R^*$ , they can be calculated with the above expressions. They are plotted in Figure 6.2 for the specific parameter set.

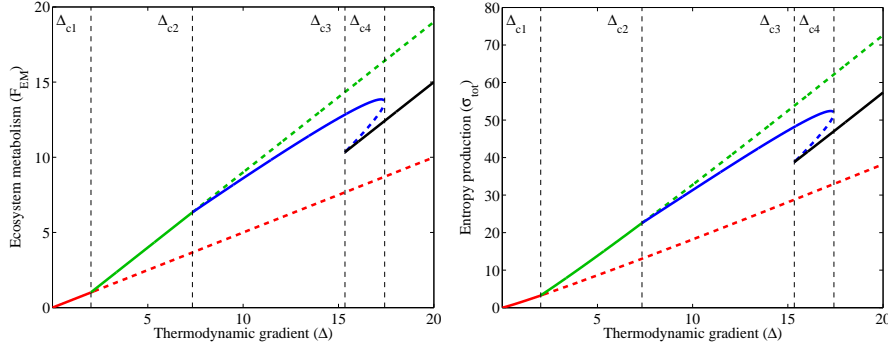


Figure 6.2: Resource-consumer-omnivore food web. Bifurcation plot of the ecosystem metabolism  $F_{EM}$  ( $\text{mol C m}^{-2} \text{ yr}^{-1}$ ) and the entropy production  $\sigma_{tot}$  ( $\mu\text{W m}^{-2} \text{ K}^{-1}$ ) at steady state as a function of the thermodynamic gradient  $\Delta$  ( $\text{kmol C m}^{-3}$ ). The dashed lines are the unstable states, the solid lines are stable states.

## 6.3 The test

We are now ready to test the different MaxEP hypotheses. Fig. 6.3 shows a close-up of fig 6.2, but for other parameter values suited for our discussion.

### 6.3.1 Non-variational MaxEP

*Is the EP of the most stable steady state the highest?* This question is relevant for determining the selected steady state when e.g. knowledge of initial conditions is lacking. It might also be applicable in the study of catastrophic regime shifts in ecosystems with multiple steady states [176].

Looking at fig. 6.3, points 'b' and 'c' correspond to the two asymptotically stable states for the same  $\Delta$ . If the gradient increases, point 'b' reaches the saddle-node bifurcation. Therefore, the stability of 'b' decreases the closer it

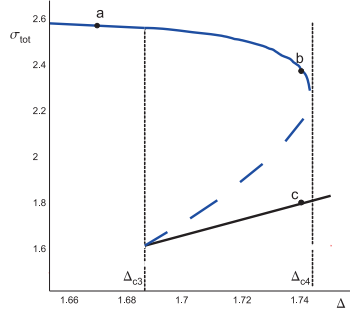


Figure 6.3: A close-up of the EP in the steady states as a function of  $\Delta$ , for parameter values  $\alpha_R = 1, g_{CR} = 25, q_{CR} = 1/5, g_{OR} = 2, q_{OR} = 1/2, g_{OC} = 100, q_{OC} = 1/10, \kappa_{AC} = 0.55, d_C = 1, d_O = 1$  and  $C_R^{eq} = 0.1$ .

gets to this bifurcation point. As the stability can get infinitesimally small, it gets smaller than the finite stability of point 'c'. But the latter has a *lower* EP. Therefore, the most stable state is not always the one with highest EP.

Note that this multistability indicates the possibility of a catastrophic regime shift: A small perturbation of the coexistence state 'b' might result in an evolution towards omnivore monoculture state 'c' (see fig. 6.1). I.e. the consumer species might suddenly go extinct even if the initial perturbation at 'b' was small. This small perturbation can therefore cause a sudden decrease in EP.

### 6.3.2 Partial steady state MaxEP

*Is the steady state ecosystem metabolism rate close to the value where the ecosystem metabolism EP is maximal?*

This formulation of the partial steady state MaxEP was presented in chapter 3 and section 5.5. It involves not the total EP, but only the ecosystem metabolism EP, given by

$$\begin{aligned}\sigma_{EM}^* &= F_{EM}^* R \ln \frac{C_R^*}{C_R^{eq}} \\ &= F_{EM}^* R \ln \left( \frac{C_R^0 - F_{EM}^*/\alpha_R}{C_R^{eq}} \right).\end{aligned}\quad (6.18)$$

This EP obtains a maximum for a specific value  $F_{EM,MaxEP}^*$ , which equals the ecosystem metabolism rate. One can quickly see that the maximum value for  $F_{EM,MaxEP}^* = F_{R,MaxEP}^*$  and  $C_{R,MaxEP}^*$  does not correspond with the explicit multiple steady state solutions above (because the MaxEP value is unique). This rejects the partial steady state MaxEP.

Although our RCO ecosystem can be seen a theoretical counterexample, in chapter 10 we will make a distinction between the macro- and the megascopic level. Our RCO system is macroscopic, and theoretical counterexamples at the much more complex megascopic level are not yet found.

### 6.3.3 Total steady state MaxEP

*Does the ecosystem EP increase under evolution?*

In chapter 3, we have seen that the total EP becomes maximal for  $\kappa_{EM} \rightarrow \infty$ . This means e.g.  $\kappa_{AC} \rightarrow \infty$  or  $g_{CR} \rightarrow \infty$ , which is always unphysical.

However, the variation of the biological parameters ( $g_{CR}$ ,  $d_C$ ,  $g_{OC}$ , ...) has some ecological relevance. Suppose that the omnivores are predators that do not feed directly on the resource (i.e.  $g_{OR} = 0$ ). When new consumer or predator species are introduced in the ecosystem, either by immigration or genetic mutation, a new stable state might be attained. Our RCP chemostat is simple enough (e.g. one resource, constant inflow, homogeneous concentrations, no time delays in the dynamics, ..., see [185]) for the famous competitive exclusion principle [7] to be valid. The consumer species with the highest fitness

$$\Phi_C \equiv q_{CR}g_{CR}/d_C, \quad (6.19)$$

survives, the other consumer species go extinct (at the condition that the predators predate equally on all consumer species). The same happens for the predator: the one with the highest fitness

$$\Phi_P \equiv q_{PC}g_{PC}/d_P \quad (6.20)$$

survives. The fitness measures for consumer or predator only depend on the biological parameters. Therefore, evolution or succession is a slow shift towards the new state, and this is mathematically speaking a slow movement in parameter space, the space spanned by the biological parameters.

With the above idea, a weaker version of this MaxEP hypothesis can be formulated: Does the EP slowly increase under evolution or succession? Fig. 6.4 shows what will happen with the total steady state EP when the consumer or predator parameters slowly change. If the consumer turns into a 'fitter' species, the EP increases, which affirms the weak MaxEP formulation<sup>2</sup>. But when the predator becomes fitter, the total EP decreases, disproving weak MaxEP.

### 6.3.4 Lyapunov EP

*What is the behavior of the EP when the ecosystem evolves from a transient to a steady state?*

This question is related with the Lyapunov EP hypothesis. As we know, close to equilibrium ( $\Delta$  small), there is MinEP:  $d\sigma/dt < 0$ . But far from equilibrium, this is not valid anymore. And as we already stressed, it is quite difficult to calculate the EP in far-from-equilibrium transient states. Therefore, we are not yet able to solve this question for ecosystems.

Our next chapter deals with ecological goal functions. As we will see, one possible definition of a goal function is that it is a Lyapunov function. Therefore, the next chapter will move on more dangerous fields, because we are going to calculate the EP and other thermodynamic quantities both for steady and transient states. Our results will be negative: under the population dynamics

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<sup>2</sup>This MaxEP is also related with the non-variational MaxEP. What we basically do is comparing the EP's for a discrete set of steady states. This set of steady states arises in an ecosystem with five variables: one resource ( $C_R$ ), two consumer species ( $C_C$  and  $C'_C$ ) and two predator species ( $C_P$  and  $C'_P$ ).

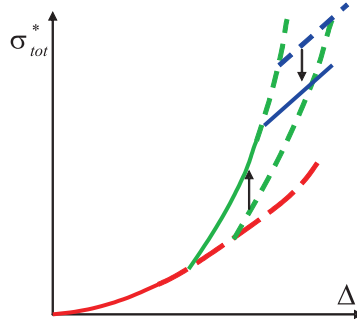


Figure 6.4: The total steady state EP for a system with two consumers and two predators. This system is used to study evolution or succession. As the two arrows indicate, consumer evolution increases the EP, whereas predator evolution decreases the EP.

of the system, the EP does not show a constant increase or decrease. Therefore, we can expect that the EP does not behave as a Lyapunov function for the population dynamics.

### 6.3.5 Gradient response

*Does the EP increase when the system is driven further out of equilibrium?*

This gradient response hypothesis might be relevant in the assessment of environmental changes in e.g. the resource feeding. It might also be relevant in the study of spatial patterns. E.g. the resource depositing in deep sea sediments is lower than at the coastlines. Therefore, coastal and estuarine sediment ecosystems are driven further out of equilibrium than deep sea sediments.

Looking at point 'a' in fig. 6.3, it is the only stable state for that specific value of  $\Delta$ . This external gradient  $\Delta$  measures the distance from equilibrium. The system is driven further out of equilibrium when the environment changes and  $\Delta$  increases.

But  $d\sigma_{tot}^*/d\Delta|_a < 0$ . The unselected unstable states have  $d\sigma_{tot}^*/d\Delta > 0$ . Therefore, both the weak and the strong gradient response hypotheses are invalid: The EP does not increase, let alone increase maximally, when the system is driven further out of equilibrium. Observe a particular behavior around point 'b'. If the ecosystem is slowly driven further out of equilibrium, we see that the EP slowly decreases, but at  $\Delta_{c4}$  there will be a sudden jump, the consumer species goes extinct (see fig. 6.1) and the EP will suddenly decrease. This jump is the consequence of an increase in resource input, i.e. a change in the *environment*. In contrast to the effect of a small ecosystem perturbation as mentioned in section 6.3.1, this jump occurs even when there are no ecosystem perturbations that drive the system out of its steady state. The ecosystem perturbation is a change in the *ecosystem* whereby the environment is kept constant.

This intriguing behavior of the EP in the omnivore ecosystem might seem a bit counterintuitive. One would expect to see an increase in irreversibility (EP) when a system is driven further out of equilibrium. Metaphorically speaking, a steeper mountain is expected to have a faster flowing river. The steepness corresponds with the driving force and the flow with the ecosystem metabolism

rate. But apparently our ecosystem behaves as a 'complex, non-linear river' with unexpected behavior.

## 6.4 Discussion: Entropy production, ecosystem stability and biodiversity

Are there relations between stability, biodiversity and EP? The discussion about stability and biodiversity of ecosystems revived in the past 30 years, basically due to the seminal work of May [113]. He studied theoretical models of 'random' food webs, and demonstrated that the more species are introduced (with random interaction strengths), the more unstable the ecosystem becomes (we refer to [113] for the mathematical notions 'random' and 'stable'). Simply stated, if one would construct an ecosystem 'blindfolded', i.e. choose the species and the predation and competition strengths randomly, then the ecosystem is more likely to crash when the number of species increases. This did not confirm some observations of stable and biodiverse ecosystems. Obviously, a real ecosystem is not constructed randomly. This motivated some theoretical ecologists to look for principles that determine the interaction strengths [115]. One branch of research is to look for organizational principles, more specifically goal functions. The next section will elaborate on these goal functions. As the EP is a candidate goal function, the relevance of the above question concerning the relation between EP, stability and biodiversity becomes clear.

However, as discussed above in section 6.3.1, the most stable steady state is not necessarily the one with the highest EP. This already criticizes the proposal that the EP is a goal function. What about the relation with biodiversity? It is often stated [179] that a system that is more complex or biodiverse has more irreversible processes, i.e. more pathways and mechanisms to degrade externally applied gradients (or to dissipate energy). In other words, if this hypothesis is correct, there should be a positive relationship between biodiversity and ecosystem EP. Let us test this hypothesis by studying theoretical Lotka-Volterra chemostat ecosystems.

We have already seen in section 6.3.1 that an ecosystem with only consumers present might have a higher EP than an ecosystem with both consumer and predator or omnivore species present. Therefore, ecosystems with longer trophic chains (and hence more species) can have lower EP's. This counters the hypothesis for trophic chain biodiversity.

But there is also trophic level biodiversity, whereby multiple species compete with each other at the same trophic level. We already mentioned the competitive exclusion principle: If multiple consumer species are competing for the same resource, only the fittest species survives. How to introduce multiple coexisting species at the first trophic level? There are different possibilities (see e.g. [185]). One possibility is the additional nutrient competition model. Suppose that there are different nutrients (e.g. nitrogen,...) necessary to drive the growth of the consumers. Suppose the growth rate of consumer species  $b$  looks like  $g_{bR} = \sum_n \gamma_{bn} C_n$ , with  $C_n$  the concentration of the  $n$ -th nutrient and  $\gamma_{bn}$  some parameters. The higher  $\gamma_{bn}$ , the less nutrient of type  $n$  is required for growth of species  $b$ . Next, suppose that the total amount of nutrients in the ecosystem remains conserved, and there is no nutrient exchange with the environment.

That means that the concentration of free nutrients is  $C_n = C_n^{tot} - \sum_b \nu_{nb} C_b$ , with  $C_n^{tot}$  the total concentration of nutrients (the maximal concentration of free nutrients). The sum means that an amount of the nutrients is taken up by the consumer species. These are bounded nutrients, and they are no longer available for biomass growth of other species. Putting everything together, we get as growth rates  $g_{bR} = g_{bR}^0 - \sum_b G_{bb'} C_{b'}$ , with  $G_{bb'} = \sum \gamma_{bn} \nu_{nb'}$  the competition matrix.

The above additional nutrient model allows to study competition between different coexisting consumers at the first trophic level. One can study stable steady states with a number of non-zero consumer populations. For these stable coexistence states, one can calculate  $C_R^*$  and consequently  $F_R^*$  and  $\sigma_{tot}^*$ . Playing around with this model, in particular with the parameters of the competition matrix, it becomes clear that there is no simple relation between the number of surviving species and the EP. Therefore, we can conclude that from a theoretical perspective, also the trophic level biodiversity does not always contribute to the EP. In summary, there are no simple relations between the trio EP, ecosystem stability and biodiversity.

## Chapter 7

# Testing ecological goal functions and efficiency measures

### Abstract

A chemotrophic resource-consumer-predator (RCP) ecosystem is described as a chemical reaction system in local equilibrium. Although comments on its degree of realism are given, the approach allows for a consistent thermodynamic description with explicit expressions for kinetic parameters, reaction rates, thermodynamic chemical potentials and affinities. With these thermodynamic and kinetic quantities, one can compose a lot of interesting ecological measures which are commonly used in the studies of the evolution, stability or (thermodynamic) efficiency of ecosystems. An important set of these ecological measures are the goal functions (ecosystem orientors), for which three different definitions are given. Next, we will give more than 30 explicit expressions (in terms of the RCP model) for goal function proposals, and these are tested with respect to the three general definitions. This can be done by solving the ecosystem dynamics or by studying the evolutionary fitness of consumers and predators. The conclusion is that all the proposals are invalid as general goal functions, because there are (physically) relevant parameter regimes where the proposals do not meet the conditions of any of the three definitions. We will also formulate more than 10 (biological or thermodynamical) efficiency measures in terms of the RCP ecosystem, and try to find relations with the other measures. No interesting non-trivial relation was found. The appendix contains a new derivation for the exergy of the ecosystem as used by Mejer and Jørgensen (1979). This alternative derivation gives some new physical interpretations of the terms that appear in the exergy function.

### 7.1 Introduction

Is it true that when organisms become more efficient in the captation of free energy, they become more able to survive? And if they are 'fitter', can they grow in numbers such that e.g. biomass, ecosystem free-energy or primary production

maximizes? And does this also result in more cycling or higher stability?

Studies relating biological efficiency with thermodynamics and ecosystem functioning already go back to the work by Lotka [99], who believed that natural selection is basically a struggle for Gibbs free energy, the energy capable to perform work. Odum [141] ignited a second boost in this field of system ecology, by proposing some ecological quantities (e.g. cycling, energy throughflow,...) that show some specific behavior (e.g. a gradual increase) under ecosystem development. Later on, the work by Odum became important in the study of (anthropogenic) disturbances in (mature) ecosystems [81, 127, 129, 179, 202]. This resulted in a huge increase of studies concerned with the search for ecological goal functions (GF). According to Ray [161], the GF is the most modern approach in theoretical ecology. Ecosystems are believed to have a self-organizing ability to cope with perturbations, and this self-organization also expresses itself as a gradual increase of a GF under ecosystem development. Therefore, ecological goal functions are known as extremal principles. Related with the notion of a GF, there is the notion of efficiency. This is an important concept in thermodynamics, but also in the study of e.g. biological growth. Efficiency is believed to increase under ecosystem evolution by genetic mutations and natural selection. The major question we will ask and try to solve is: Is there a non-trivial relation between ecosystem evolution, efficiency and some proposed goal function?

The previous chapters had their primary focus on the entropy production. As the growing MaxEP literature suggests, EP is believed to be a good candidate for an extremal principle (i.e. a goal function). However, chapter 6 contains some criticism on this MaxEP proposal. The present chapter will focus primarily on the other GF proposals made in the literature. The search for and experimental testing of goal functions, as well as the search for complementarities and relationships between the different GF proposals [61, 136], has received much attention in recent years.

However, there is a lot of confusion in this subfield of theoretical ecology. Not only do goal functions live under various different names ('eco-targets', 'extremal principles', 'organizational principle', 'ecosystem orientors', 'ecological imperatives' or 'maturity indicators' are all used), they are also often quite vague and ambiguous. What do we mean by ecosystem development, and how to model it? The latter question is related with time-scales: Does ecosystem development refer to population dynamics (whereby the number of individuals can change, but the number of species can not increase), to succession or to slow evolution (where an increase in the number of species is possible due to mutations)? As we explore the literature, we basically encounter different meanings, with different applications. Therefore, we first have to define a goal function. It appears that there are three possible definitions which might be relevant. These definitions are very much related to some hypotheses in the EP classification in chapter 5.

But not only the definition of a GF itself was too vague. Also specific proposals (such as exergy, specific dissipation, empower,...) are not always well defined. We have the same situation with the notion of efficiency. We can define different efficiencies, based on thermodynamical (Carnot efficiency, first law efficiency,...) or kinetic (flow efficiency, cycling efficiency,...) quantities. For explicit mathematical expressions of proposed goal functions and efficiencies, we need a tangible mathematical ecosystem model.

We will study a resource-consumer-predator (RCP) generalized Lotka-Volterra chemostat ecosystem, in much the same way as in chapters 4 and 6. However,

there is one big 'extra' of the model in this chapter: In order to write down expressions for some GF's and efficiencies, we need to refine our ecosystem description, because the thermodynamic problems mentioned in chapter 2 will become very acute. As argued by Pross [160], we have to make the important distinction between thermodynamics and kinetics. The basic thermodynamic problem is related with the calculability of the free energy of the ecosystem or the chemical potentials of organisms. The basic kinetic problem is related with the flux expressions: If the thermodynamic quantities are well defined, the fluxes can not be arbitrary because e.g. the second law of thermodynamics implies that the entropy production should be positive. Furthermore, from a thermodynamic point of view, every process (e.g. biological growth) has an inverse process which might be highly unlikely, but never has zero probability.

Both thermodynamic and kinetic problems can be solved in our approach, which lies in a reformulation of the RCP ecosystem as if it were a chemical reaction system of ideal solutions of chemicals (including organisms) with elementary reactions obeying mass action kinetics. Unrealistic as it may seem, with this 'chemical' RCP model, rigorous definitions of the GF proposals can be written down. Finally, when every definition of every quantity is clarified, the next, big game begins: the search for relations between the more than 30 goal functions and the more than 10 efficiency measures. We did not find any non-trivial relations, and none of the proposed GF's did satisfy any of the three definitions of a GF in all relevant parameter regimes (this result is in line with the more abstract argumentation in [207]). As a consequence, some statements in the literature will be tackled.

## 7.2 Definitions for goal functions

We can give at least three different definitions of an ecological goal function  $Gf$ . Mathematically it is a function on the state space  $\Gamma$  (e.g.  $\Gamma = \mathbb{R}_+^N$ , with coordinates the different (abiotic or biotic) concentrations  $C_p$ ,  $p = 1, \dots, N$ ), and it is also a functional on  $\mathbb{R}$  because the coordinates of  $\Gamma$  are variables, i.e. they are functions of time  $t \in \mathbb{R}$ . Furthermore, the goal function might depend on a set of parameters  $\{\pi_\alpha\}$  appearing in the dynamics. The goal function  $Gf(\{C_p\}, \{\pi_\alpha\})$  can be defined in at least three ways:

### 7.2.1 Lyapunov goal function

Under short time-scale population dynamics, the goal function should obey

$$\frac{dGf}{dt} \geq 0. \quad (7.1)$$

In mathematical terminology, this is called a Lyapunov functional. (A weaker condition consists of  $Gf \leq Gf^*$  for all time, and  $Gf_{t \rightarrow \infty} = Gf^*$ ). The population dynamics means that the number of species (and hence the dimension of the state space) does not increase. This definition is the same as the Lyapunov EP described in section 5.7.

## 7.2.2 Steady state goal function

Suppose the system is in the steady state<sup>1</sup> (denoted with  $*$ ) for the ecological dynamics. That means that the variables  $C(t)^*$  become time-constants and functions of the parameter(s)  $\pi_\alpha$ . However, ecosystems have also a much longer timescale, the evolutionary time scale  $\tau \gg t$ . For this timescale, the parameter(s) might very slowly change from  $\pi_\alpha$  to  $\pi'_\alpha$ , due to mutation and natural selection<sup>2</sup>. This results into a very slow shift of the steady state. The goal function should satisfy  $Gf(C^*(\pi)) \leq Gf(C^*(\pi'))$ , or for small increases in  $\pi_\alpha$ :

$$\frac{dGf(\pi)}{d\tau} \geq 0. \quad (7.2)$$

This definition is the same as the steady state MaxEP in sections 5.5, 5.6, 6.3.2 and 6.3.3. As (7.2) shows, this definition is a Lyapunov principle for evolutionary time-scales. The GF is a Lyapunov function on parameter space.

## 7.2.3 Non-variational goal function

If there are multiple steady states, and one considers a bifurcation diagram dependent on a parameter (e.g. in our ecosystem it could be the gradient  $\Delta$ ), one would like to have a criterium which one of the states is most stable. The asymptotic (linear) stability can be measured by the resilience  $R \equiv -\max(\text{real}(\zeta))$ , where  $\zeta$  are the eigenvalues of the linearized system. The goal function can serve this criterium if its steady state value obeys

$$Gf|_{\text{most stable}}^* \geq Gf|_{\text{less stable}}^*. \quad (7.3)$$

If the inequality is invalid, to say that an ecosystem wants to maximize its goal function means to say that it chooses for a less stable or unstable state, which is less realistic or even unrealistic. This definition is the same as the non-variational MaxEP in section 5.4.

So a goal function can be defined in at least three possible ways, but note that the former two definitions are variational principles and the latter is not because it is a selection principle that selects the 'real' state amongst a discrete set of steady states. The difference in the former two is due to a different time scale, as was mentioned in [207] and section 5.7. It is also important to note that in our modeling the structure of the food web remains the same. Changing food webs have a changing dimension of the state space  $\Gamma$ . It remains an unsolved problem how to define quantitatively a goal function for changing food webs, and how to test goal function proposals in those models.

<sup>1</sup>When there are time dependent attractor states (periodic, pseudo periodic or chaotic states), one can take suitable time averages.

<sup>2</sup>Stated more correctly, after a mutation of an 'old' species (with concentration  $C_p$ ), a new species appears, with new variable ( $C'_p$ ). So the dimension  $N$  of the state space is increased to  $N + 1$ . However, in the simple chemostat models that we will study, due to the competitive exclusion principle [7], the weakest species eventually goes extinct (see section 6.3.3). Therefore, the final steady state can be projected onto a  $N$  dimensional state space because one variable ( $C_p$  or  $C'_p$ ) becomes zero.

## 7.3 General set-up and thermodynamic problems

Having defined a GF, we are now going to move to the RCP chemostat ecosystem model (see chapter 2). The resource flows into the ecosystem where a consumer-predator trophic chain degrades the resource into waste products. The four compartments are the homogeneous concentrations of the various abiotic and biotic species  $C_p$ , with  $p = R, C, P$  or  $W$  for resp. resource, consumer, predator and waste products. These are the system variables. The number of 'elementary' molecules<sup>3</sup> in the different compartments of the system are written as  $N_p = V^{sys} C_p$ , and for the environment  $N_p^0 = V^{res} C_p^0 \approx \infty$ , with  $V^{sys}$  and  $V^{res} \approx \infty$  the volumes of respectively system and environmental reservoirs.

When studying the thermodynamics of this RCP ecosystem, there are two difficult problems. One is related with thermodynamics: the state functions (entropy, free energy) and the intensive quantities (chemical potentials). The other is related with kinetics: the fluxes (transport and reaction rates).

### 7.3.1 Problems with thermodynamic quantities

One often needs to know the free energies (or chemical potentials) of the abiotic and biotic compartments in order to measure their 'energetic quality' (we refer to [88] for detailed elaborations). However, we now know that it is highly difficult to correctly measure or calculate these free energies of complex organisms. Indeed, it is even an existential question whether these quantities ever exist. To deal with this issue, we will apply strong simplifications as we proceed.

First, for systems at constant and homogeneous pressure  $p$  and temperature  $T$ , we can look at the Gibbs free energies  $G_p$ , which are related to the chemical potentials as

$$\mu_p(p, T, N) = (\partial G_{tot}^{sys} / \partial N_p)_{N_{q \neq p}, T, p} \quad (7.4)$$

with the total system free energy  $G_{tot}^{sys}$  as the sum of the free energies of all substances within the system. The variation is performed with constant  $N_{q \neq p}$ ,  $T$  and  $p$ .

Some goal function or efficiency measures we will encounter later on only depend on the chemical potentials of resource and waste. If we assume for modeling simplicity that resource and waste are ideal and perfect solutions, then we can write  $\mu = \mu^r + RT \ln C$ , with  $R$  the ideal gas constant and  $\mu^r$  the reference chemical potentials for unit concentration. But some measures used in the literature depend on the free energies of the biotic compartments as well. As nobody knows the correct expressions for these free energies, the best we can do for the moment is to make a very strong simplification: We assume that the biotic compartments have free energies (chemical potentials) as if they were ideal solutions. This expression is plainly wrong for real systems, but for a first approximation in a theoretical model with emphasis on the qualitative behavior,

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<sup>3</sup>Note that one biotic organism can have many 'elementary' molecules and that the biotic concentrations are the number of elementary molecules (not individual organisms) per unit volume. In our chemo-heterotrophic ecosystem model, the elementary molecules of the organisms are the resource molecules. The latter are therefore the basic building blocks of the biomass. The concentration of individual organisms is given by  $C'_b = C_b/a_b$ , with  $a_b$  the number of elementary molecules.

we will take it for granted in this article. The biotic chemical potentials appear explicitly in the following quantities that we will encounter later on:

- The exergy (including the exergy specific dissipation, the benefit/cost and the emergy/exergy ratios),
- the entropy or heat production of a specific biotic reaction<sup>4</sup> and
- all the thermodynamic efficiencies (except the chemical Carnot efficiencies).

This list is the set of quantities that have a weak spot: As they explicitly depend on the biotic chemical potentials, one should be cautious not to take our obtained results that involve these quantities too realistically.

### 7.3.2 Problems with kinetics

The second type of problems deal with the fluxes between the different compartments. The difficulty is that we want to use flux expressions which are (approximately) the ones used in ecological models, but we also want thermodynamic consistency. The best strategy is to describe the food web functioning in terms of reactions, as if the system was an ordinary chemical reaction system. In thermodynamics, every non-zero forward flux (forward reaction rate)  $F_{\rightarrow}$  has a corresponding non-zero backward flux  $F_{\leftarrow}$ , so the net flux is  $F = F_{\rightarrow} - F_{\leftarrow}$ . In chemical reaction systems, each net flux has a thermodynamic conjugate force  $X = -A/T$  with  $A$  the affinity of the reaction. The affinities are the differences of the chemical potentials of the compartments involved in the reactions, weighted by their stoichiometric coefficients (the coefficients in the reaction equations) [88].

The flux expressions are not completely independent from the force expressions, because otherwise the second law of thermodynamics, the positivity of the entropy production, might be violated. In this respect, some flux parameters might be related with e.g. the  $\mu^r$ . The simplest way to proceed, is by making another strong simplifications which guarantees consistency at the cost of being less realistic. The fluxes will have expressions as if they would obey mass action kinetics [88], which means that the forward and backward fluxes are the products of the involved concentrations with the stoichiometric coefficients as powers. This also means that the system functions as if it would have (composite) elementary reactions, i.e. reactions with the special property that  $X \propto \ln(F_{\rightarrow}/F_{\leftarrow})$ . The latter clearly indicates that, as mentioned above, the backward rates can not be zero when the forward rates are non-zero. At first sight, this contradicts the knowledge in biology: the non-zero backward rate of the biotic mortality indicates that there is spontaneous emergence of organisms out of low quality abiotic waste products, which is not observed. But thermodynamically there is a very small probability that life spontaneously emerges out of waste. So, the backward fluxes are so small that they can be neglected in the flux expressions ( $F \approx F_{\rightarrow}$ ), but not in the logarithm of the force expression. (Take e.g.  $F_{\rightarrow}/F_{\leftarrow} = \mathcal{O}(10^{100})$ . Then  $X = \mathcal{O}(100)$ , which is a reasonable number, even when  $F_{\leftarrow}$  is very low.)

<sup>4</sup>In chapters 2 and 3, we have seen that the mixing EP, the quasi steady state ecosystem metabolism EP and the steady state total EP did not explicitly depend on the biotic chemical potentials.

## 7.4 The resource-consumer-predator model

The above discussion might sound abstract, but it will become more concrete in the specific RCP ecosystem example. Let basics of the model were discusses in chapters 2 and 4.

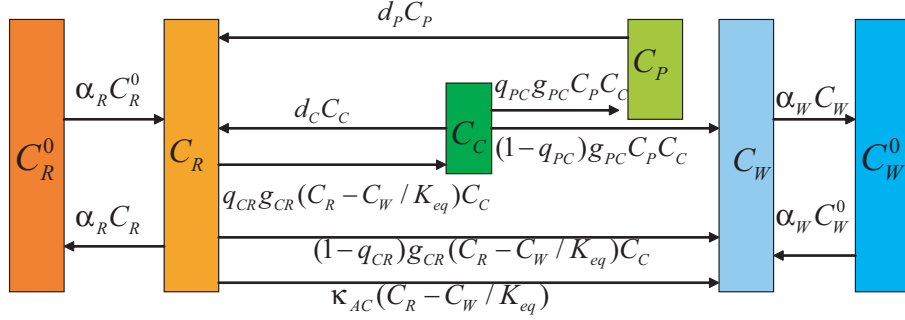


Figure 7.1: The ecosystem foodweb with the six carbon compartments and the flows between them.

### 7.4.1 The kinetics

The above reactions, as well as the exchanges of resource and waste with the two environments, obey some kinetics. These kinetics are completely given by the fluxes. The backward fluxes (obeying mass action kinetics) are in biological reactions very very small, but for completeness, we shall include them here, and simplify the expressions later on, such that the ecosystem fluxes as used in chapter 4 and fig. 7.1 are obtained. In other words, we will demonstrate that the expressions for the ecosystem fluxes that we used in previous chapters are justified as being limiting cases of the chemical reaction fluxes.

The list of the exchange and chemical reaction fluxes (in 'mass action kinetics' formulation) is:

- Exchange (in- and outflow) of resource with the external resource reservoir

$$F_R = \alpha_R(C_R^0 - C_R). \quad (7.5)$$

- Exchange (in- and outflow) of waste with the external waste reservoir

$$F_W = \alpha_W(C_W - C_W^0). \quad (7.6)$$

- The abiotic conversion

$$F_{AC} = \kappa_{AC}C_R - \kappa_{AC}^{\leftarrow}C_W. \quad (7.7)$$

We write the equilibrium constant as  $K_{eq} \equiv \kappa_{AC}/\kappa_{AC}^{\leftarrow}$  and the equilibrium resource concentration as  $C_R^{eq} \equiv C_W/K_{eq}$ .

- The consumer growth (syn.: consumer resource uptake)

$$F_{gCR} = g_{CR}C_C C_R - g_{CR}^{\leftarrow}C_C^{1+q_{CR}}C_W^{1-q_{CR}}. \quad (7.8)$$

Here we have made the assumption that the growth reaction has the kinetics of mass action<sup>5</sup>.

- The consumer decay (syn.: consumer biomass turn-over)

$$F_{dC} = d_C C_C - d_C^- C_R. \quad (7.9)$$

- The predator growth (syn.: predator consumer uptake)

$$F_{gPC} = g_{PC} C_C C_P - g_{PC}^- C_P^{1+q_{PC}} C_W^{1-q_{PC}}. \quad (7.10)$$

- The predator decay (syn.: predator biomass turn-over)

$$F_{dP} = d_P C_P - d_P^- C_R. \quad (7.11)$$

These are the kinetic expressions that appear in the dynamical equations that will be presented in a later section. For later use, we also need to define a few extra rates, related with anabolism and catabolism:

- The consumer anabolic rate  $F_{aC} \equiv q_{CR} F_{gCR}$  (syn.: consumer biomass synthesis),
- The predator anabolic rate  $F_{aP} \equiv q_{PC} F_{gPC}$ ,
- The consumer catabolic rate  $F_{cC} \equiv (1 - q_{CR}) F_{gCR}$  (syn.: consumer biotic conversion),
- The predator catabolic rate  $F_{cP} \equiv (1 - q_{PC}) F_{gPC}$ ,

### 7.4.2 The thermodynamics

In a previous section we have discussed our strategy to take all compartments as if they were ideal and perfect solutions in water. This simplifies the chemical potential expressions. In our strategy we also imposed flux expressions as if they would correspond with elementary reactions. Therefore, the affinities  $A = TX$ , related with the thermodynamic forces  $X$ , for all the exchanges and chemical reactions are given by:

- Exchange (in- and outflow) of resource with the external resource reservoir

$$A_R = \mu_R - \mu_R^0 = -RT \ln \frac{C_R}{C_R^0}. \quad (7.12)$$

- Exchange (in- and outflow) of waste with the external waste reservoir

$$A_W = \mu_W - \mu_W^0 = -RT \ln \frac{C_W}{C_W^0}. \quad (7.13)$$

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<sup>5</sup>Note that this mass action kinetics is purely formal: As  $q_{CR} \leq 1$  is not necessarily an integer, the above expression does not follow from simple considerations about random molecular collisions. We will not go into a 'microscopic' derivation for the choice of kinetics.

- The abiotic conversion

$$\begin{aligned} A_{AC} &= \mu_W - \mu_R \\ &= -RT \ln \frac{\kappa_{AC} C_R}{\kappa_{AC}^- C_W}. \end{aligned} \quad (7.14)$$

- The consumer growth

$$\begin{aligned} A_{gCR} &= q_{CR} \mu_C + (1 - q_{CR}) \mu_W - \mu_R \\ &= -RT \ln \frac{g_{CR} C_C C_R}{g_{CR}^- C_C^{1+q_{CR}} C_W^{1-q_{CR}}}. \end{aligned} \quad (7.15)$$

- The consumer decay

$$\begin{aligned} A_{dC} &= \mu_R - \mu_C \\ &= -RT \ln \frac{d_C C_C}{d_C^- C_R}. \end{aligned} \quad (7.16)$$

- The predator growth

$$\begin{aligned} A_{gPC} &= q_{PC} \mu_P + (1 - q_{PC}) \mu_W - \mu_C \\ &= -RT \ln \frac{g_{PC} C_C C_P}{g_{PC}^- C_P^{1+q_{PC}} C_W^{1-q_{PC}}}. \end{aligned} \quad (7.17)$$

- The predator decay

$$\begin{aligned} A_{dP} &= \mu_R - \mu_P \\ &= -RT \ln \frac{d_P C_P}{d_P^- C_R}. \end{aligned} \quad (7.18)$$

A few remarks are in order.

- The affinity for the consumer and predator growth are now consistent with the mass action kinetics we have chosen.
- The backward rates can not be neglected in the affinities.
- In order that every reaction occurs spontaneously in the positive direction ( $F > 0$ ),  $A$  should be negative.

For later use, we also need some additional affinity definitions:

- The anabolic consumer affinity  $A_{aC} \equiv \mu_C - \mu_R = -A_{dC}$ ,
- The anabolic predator affinity  $A_{aP} \equiv \mu_P - \mu_C$ ,
- The catabolic consumer affinity  $A_{cC} \equiv \mu_W - \mu_R$
- The catabolic predator affinity  $A_{cP} \equiv \mu_W - \mu_C$

With all the definitions of kinetic parameters, rates, chemical potentials and affinities, one can rigorously define a lot of measures, used to study the evolution, stability or efficiency of ecosystems. This will be done in a later section, but first we will study the full dynamics and the steady state solutions.

### 7.4.3 The dynamical equations and the steady state solutions

In order to derive the dynamical equations, we will first simplify the reaction rates. This will be done in Appendix 7.10. This results into the following dynamical equations for the variables  $C_R$ ,  $C_C$ ,  $C_P$  and  $C_W$ :

$$\begin{aligned} \frac{d}{dt}C_R &= \alpha_R(C_R^0 - C_R) - (\kappa_{AC} + g_{CR}C_C)(C_R - C_W/K_{eq}) \\ &\quad + d_C C_C + d_P C_P, \end{aligned} \quad (7.19)$$

$$\frac{d}{dt}C_C = q_{CR}g_{CR}(C_R - C_W/K_{eq})C_C - g_{PC}C_C C_P - d_C C_C, \quad (7.20)$$

$$\frac{d}{dt}C_P = q_{PC}g_{PC}C_C C_P - d_P C_P, \quad (7.21)$$

$$\begin{aligned} \frac{d}{dt}C_W &= \alpha_W(C_W^0 - C_W) + (\kappa_{AC} + (1 - q_{CR})g_{CR}C_C)(C_R - C_W/K_{eq}) \\ &\quad + (1 - q_{PC})g_{PC}C_C C_P \\ &\approx 0 \quad (\rightarrow C_W \approx C_W^0). \end{aligned} \quad (7.22)$$

These equations are the well known chemostat equations (see e.g. [185]) we encountered more generally in chapter 4<sup>6</sup>. We will take infinite waste exchange ( $\alpha_W \rightarrow \infty$ ) for simplicity. (A finite waste exchange will give the same qualitative behavior.)

The chemostat ecosystem has the compartment-flux structure visualized in Fig. 7.1. One can write down the network throughflow matrix  $F_{pq}$  giving the total flux of the variable ecosystem compartment  $q$  to compartment  $p$ :

$$F = \begin{pmatrix} 0 & d_C C_C & d_P C_P & \frac{\kappa_{AC} C_W}{K_{eq}} \\ q_{CR}g_{CR}(C_R - \frac{C_W}{K_{eq}})C_C & 0 & 0 & 0 \\ 0 & q_{PC}g_{PC}C_C C_P & 0 & 0 \\ (1 - q_{CR})g_{CR}(C_R - \frac{C_W}{K_{eq}})C_C + \kappa_{AC} C_R & (1 - q_{PC})g_{PC}C_C C_P & 0 & 0 \end{pmatrix} \quad (7.23)$$

To study the steady states, the key parameter is the so called thermodynamic gradient

$$\Delta = C_R^0 - C_W^0/K_{eq}, \quad (7.24)$$

as this will be a bifurcation parameter. There are at most three steady states, one (globally) stable, and two unstable (or unphysical by having negative concentrations). Bifurcations occur at two values of the thermodynamic gradient

$$\Delta_{c1} \equiv \frac{(\alpha_R + \kappa_{AC})d_C}{\alpha_R q_{CR} g_{CR}}, \quad (7.25)$$

$$\Delta_{c2} \equiv \frac{d_C((\alpha_R + \kappa_{AC})q_{PC}g_{PC} + (1 - q_{CR})q_{CR}d_P)}{\alpha_R q_{CR} g_{CR} q_{PC} g_{PC}}. \quad (7.26)$$

<sup>6</sup>Note that thermodynamic consistency and our applied simplification naturally results in the growth rate dependence  $g_{CR}C_C)(C_R - C_W/K_{eq})$ , including the term  $-C_W/K_{eq}$ . In previous chapters, this extra term was included rather ad hoc, without much justification, except that the growth should stop in equilibrium ( $C_R = C_W/K_{eq}$ ).

Accordingly, one can define three ranges, for which the stable steady state concentrations (denoted with an asterisk) of resource, consumer and predator can be calculated.

Range  $\mathcal{R}_1$ :  $0 \leq \Delta \leq \Delta_{c1}$ :

$$C_R^* = C_R^{eq} + \frac{\alpha_R \Delta}{\alpha_R + \kappa_{AC}}, \quad (7.27)$$

$$C_C^* = 0, \quad (7.28)$$

$$C_P^* = 0. \quad (7.29)$$

Range  $\mathcal{R}_2$ :  $\Delta_{c1} \leq \Delta \leq \Delta_{c2}$ :

$$C_R^* = C_R^{eq} + \frac{d_C}{q_{CR}g_{CR}}, \quad (7.30)$$

$$C_C^* = \frac{q_{CR}g_{CR}\alpha_R\Delta - (\alpha_R + \kappa_{AC})d_C}{d_Cg_{CR}(1 - q_{CR})}, \quad (7.31)$$

$$C_P^* = 0. \quad (7.32)$$

Range  $\mathcal{R}_3$ :  $\Delta_{c2} \leq \Delta$ :

$$C_R^* = C_R^{eq} + \frac{q_{PC}g_{PC}\Delta + d_Cd_P(1 - q_{PC})}{g_{PC}q_{PC}(\alpha_R + \kappa_{AC}) + g_{CR}d_P(1 - q_{PC}q_{CR})}, \quad (7.33)$$

$$C_C^* = \frac{d_P}{q_{PC}g_{PC}}, \quad (7.34)$$

$$C_P^* = \frac{q_{CR}g_{CR}(C_R^* - C_R^{eq}) - d_C}{g_{PC}}. \quad (7.35)$$

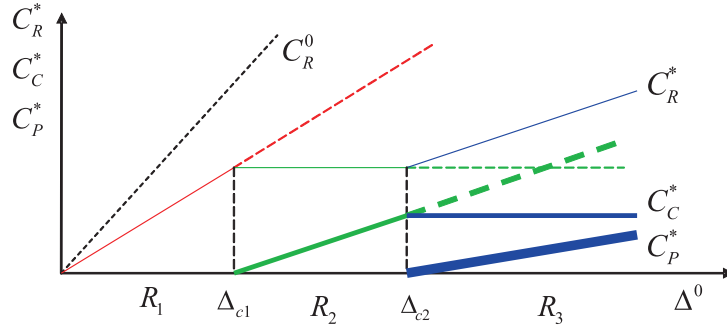


Figure 7.2: The steady state concentrations  $C_R^0$  (dotted line),  $C_R^*$  (thin line),  $C_C^*$  (thick line) and  $C_P^*$  (thickest line) as functions of  $\Delta$ . Dashed lines are unstable states, solid lines are stable.

In fig. 7.2, the steady state concentrations are given in term of the external driving force  $\Delta$  for specific parameter values. First there is a range  $\mathcal{R}_1$  with no life at all, then there is a second range  $\mathcal{R}_2$  with a monoculture of only consumers, and finally a third range  $\mathcal{R}_3$  with both consumers and predators present. The above solutions can be used to test the steady state and non-variational goal functions and efficiency measures.

In the discussion of the steady state goal function, we mentioned the importance of the competitive exclusion principle to study the behavior of the

ecosystem under evolution by natural selection. Both the consumer and the predator have an **evolutionary fitness measure**

$$\Phi_C \equiv q_{CR}g_{CR}/d_{CR}, \quad (7.36)$$

$$\Phi_P \equiv q_{PC}g_{PC}/d_{PC}. \quad (7.37)$$

If there are multiple consumer species present, and if all have the same predation loss, the one with the highest fitness  $\Phi_C$  survives and the other consumer species goes extinct. The same happens for the predators at the second trophic level: when all predator species have the same preying strength on the primary consumer, the fittest predator species survives.

## 7.5 Goal function proposals

We are now going to write expressions for the vast amount of goal function proposals studied in the theoretical ecology literature. These GF's are written down for our specific RCP ecosystem.

### 7.5.1 Kinetic goal function proposals

Here we present a number of candidate kinetic goal functions for the chemostat ecosystem. The advantage of these goal functions is that they do not depend on the thermodynamic quantities, which are as we have seen quite tricky to determine for biological organisms.

Biomass was one of the first proposals for a goal function [109]. Intuitively it is the most appealing one, but it is nowadays only used as a very rough proxy because it is believed to be of less validity. One can make a distinction between **living biomass**

$$B_{liv} \equiv C_C + C_P \quad (7.38)$$

or **total biomass** (total system storage), which includes the dead organic matter  $C_R$

$$B_{tot} \equiv C_R + C_C + C_P. \quad (7.39)$$

Next, the **consumer production** is defined by

$$P_C \equiv q_{CR}g_{CR}C_{CR}(C_R - C_W^0/K_{eq}), \quad (7.40)$$

and this is basically the anabolic flux  $F_{aC}$ .

With these, the **consumer specific production** is given by the production/biomass ratio  $P_C/C_C$ . The **predator (specific) production** can be defined in the same way.

The **residence time** for energy was proposed as a goal function by Cheslak et al. [34]. As energy is associated with the biomass, we define here the biomass residence time (the average amount of time that a carbon atom stays in biomass) for compartments  $b = C$  or  $P$  as:

$$\tau_b = \frac{C_b}{\sum_{p=R,C,P,W} F_{pb}} \quad (7.41)$$

with  $\sum_p F_{pb}$  the total outflow to all other compartments (see (7.23)). The biotic, average residence time is

$$\tau_{av} = \frac{\sum_{b=C,P} C_b \tau_b}{\sum_{b=C,P} C_b}, \quad (7.42)$$

i.e. it is the average of the individual residence times, weighted by the concentrations.

The **system import** (which is proportional with the energy capture [139]) is:

$$SI \equiv F_R = \alpha_R(C_R^0 - C_R). \quad (7.43)$$

and the **system export**:

$$SE \equiv \sum_{p=R,C,P,W} F_{4p} = F_{AC} + F_{cC} + F_{cP}. \quad (7.44)$$

The latter equals the total system respiration. The **biotic respiration** is  $R_B \equiv SE - \kappa_{AC}(C_R - C_W^0/K_{eq})$ .

The **respiration/biomass ratio** [35] can be defined by  $R_B/B_{liv}$ .

The **cycling ratio** as used by e.g. Volk [201] is

$$Cyc \equiv \frac{\sum_{b=C,P} d_b C_b + \alpha_R C_R^0 + \kappa_{AC} C_W/K_{eq}}{\alpha_R C_R^0 + \kappa_{AC} C_W/K_{eq}}. \quad (7.45)$$

When this number is e.g. 10, this means that on average out of 10 resource molecules, 1 came from abiotic sources ( $C_R^0$  and  $C_W$ ) and 9 came from biotic sources ( $C_C$  and  $C_P$ ). As these biotic organisms take up the resource and eventually recycle it by decaying, it is clear that Cyc is a good cycling ratio.

### Stability measures

Resilience and reactivity are two related notions, and they are only well defined for steady states (so one can not apply these to study the Lyapunov goal function behavior).

**Resilience** is an (asymptotic) stability measure and is defined as

$$Res \equiv -\max(\text{real}(\zeta(A))), \quad (7.46)$$

where  $\zeta(A)$  are the eigenvalues the matrix  $A_{lin}$  of the linearized system around a steady state. It is proposed by Cropp et al. [43] as an ecosystem indicator.

The notion of **reactivity** became important in the ecology literature only in the last decade [129].

$$Reac \equiv -\max\{\lambda(H(A))\}, \quad (7.47)$$

where  $\lambda(H(A))$  are the eigenvalues of the matrix  $H = (A + A^T)/2$ , the symmetric part of the matrix  $A$ . Whereas the resilience describes the asymptotic, 'late time' behavior, the reactivity describes the 'early time' behavior. Roughly speaking, when e.g.  $Res > 0$  and  $Reac < 0$ , a very small perturbation away from the steady state will initially result in an increasing deviation away from this steady state, but finally, the system evolves back towards the steady state, because it is asymptotically stable. We refer to [129] for more details.

## Network goal functions

Network goal functions are a special set of kinetic goal functions, related to the ecological food web structure [153, 154, 198]. With the throughflow matrix (7.23), one can construct important goal function proposals.

The **total system throughput** [61, 153] is naturally given by

$$TST \equiv \sum_{pq} F_{pq}. \quad (7.48)$$

The **network capacity** is:

$$NC \equiv \sum_{pq} \frac{F_{pq}}{\sum_{p'q'} F_{p'q'}} \ln \frac{F_{pq}}{\sum_{p'q'} F_{p'q'}}. \quad (7.49)$$

The **ascendency** proposed by Ulanowicz [198] is:

$$Asc \equiv \sum_{pq} F_{pq} \ln \left( \frac{F_{pq} \sum_{p'q'} F_{p'q'}}{\sum_r F_{pr} \sum_s F_{sq}} \right). \quad (7.50)$$

Roughly speaking, these quantities measure some information content of the ecosystem network, i.e. information theoretical concepts are applied to the food web. NC is a kind of Shannon information entropy<sup>7</sup> of a probability measure  $\frac{F_{pq}}{\sum_{p'q'} F_{p'q'}}$  related to the throughflow. In other words, it measures the complexity of the food web, and as some ecologists believe, the complexity of food webs increase under ecosystem development. Therefore, NC might be a relevant goal function. We refer to [61, 153] and [198] for more justifications of these expressions.

### 7.5.2 Thermodynamic goal function proposals

Let us now look at the thermodynamic goal function proposals. The advantage of these is that they are interesting from a physical point of view, because some thermodynamic measures behave as goal functions for e.g. isolated and open close to equilibrium systems. Furthermore, ecosystems are physical systems that should obey the laws of thermodynamics. If one or a few of the proposals would be valid as ecological goal function, this might open up a new perspective on the relation between physics and ecology. But as mentioned, the major disadvantage is that some (luckily not all) of them are hard to define for far from equilibrium systems.

#### Entropy production

In the previous chapters we studied the EP for generalized Lotka-Volterra chemostat ecosystems. Therefore, we will be very brief here. The new aspect of this chapter is that we can write down the EP for every independent reaction, which is given by the product of the flux (rate) with the force (affinity) [88]:

$$\sigma_{reaction} = - \frac{F_{reaction} A_{reaction}}{T} \quad (7.51)$$

---

<sup>7</sup>The Shannon information entropy  $S_I$  is a measure of 'randomness'. Take a probability measure  $p_i$ , whereby  $i = 1..N$  represents the individual stochastic outcomes and  $\sum_i p_i = 1$ . Then  $S_I \equiv - \sum_i p_i \ln p_i$ . It is maximal when the probability measure is uniform ( $p_i = 1/N$ ), i.e. maximally random.

Summing up all the reaction EP's together with the mixing EP's (see chapter 3) gives the total EP  $\sigma_{tot}$ . The nice property is that the total EP in the steady state EP's does not depend on the biotic thermodynamic quantities, nor on the choice of the kinetics (mass action, elementary reactions,...). But having explicit expressions for the affinities, we are now also able to study  $\sigma_{tot}$  in the transient states. Therefore, the Lyapunov goal function definition can be tested.

Another proposed goal function is the **biomass specific dissipation** (the biomass specific total entropy production). It is given by the total EP, divided by the living biomass  $C_C + C_P$ , and hence it is only defined in regions two and three. Alternative, one can divide by the total biomass  $C_R + C_C + C_P$  to obtain a quantity defined in all regions. Finally, Ludovisi et al. [101, 102] studied the **exergy specific dissipation**, which is defined as the EP divided with the exergy, the notion defined in the next section.

## Exergy

The **exergy** or **available energy** is one of the most frequently used ecological indicators [15, 16, 80, 81, 116]. It is a measure of how far the system is out of thermodynamic equilibrium. More specifically, it is the maximum amount of work a system can deliver when it is brought to thermodynamic equilibrium with its environment<sup>8</sup>.

Here, exergy can be defined as the difference between the total free energy (of system plus environment), with the reference total free energy when the system is in thermodynamic equilibrium with the environment. However, there is a tricky point in this definition, because we have seen that an essential feature of an ecosystem is that the environment itself is not in (internal) equilibrium. The environment should consist out of at least two environmental reservoirs that are not in mutual equilibrium, otherwise one would not be able to create a thermodynamic driving force (an energy gradient) that keeps the ecosystem operating far from equilibrium.

So when we speak about thermodynamic equilibrium, this also implies the equilibration of the environment. In our model, equilibrating the two reservoirs can be done in an infinite amount of ways. Environmental equilibrium sets in when  $C_R^0 = C_W^0/K_{eq}$ , but this does not determine the value of  $C_R^0$  itself. For the calculation of the exergy, the initial non-equilibrium state should be compared with the final equilibrium reference state, so we should transform the environment from the non-equilibrium to the equilibrium state. This can be done by e.g. increasing the waste concentration to make it equivalent with the resource concentration, or by decreasing the resource concentration, or combinations of both. In other words, there is an arbitrariness in the expression for the exergy. We believe it is most natural to let  $C_R^0$  decrease (or to decouple the resource reservoir from the system) and to keep  $C_W^0$  constant, because in realistic ecosystems the latter is related with the atmosphere  $CO_2$  concentration, i.e. it is the largest reservoir which is the most difficult to change or to decouple. This decoupling procedure is mathematically expressed as  $\alpha_R \rightarrow 0$  (keeping  $\alpha_W$  infinite),

<sup>8</sup>Recently a redefinition of the exergy concept for ecosystems was proposed, calling it eco-exergy [189]. The latter has a crucial dependence on the information stored in the system. This information is stored into the food web structure, but more so in the individual organisms, specifically its DNA/RNA structures. Our model is not able to deal with these information measures, so we will work only with exergy and not with eco-exergy.

which can also be done rather easily in laboratory chemostat experiments.

As was first derived by Mejer et al. [116], the exergy is:

$$Ex \equiv G_{tot} - G_{tot}^{eq}, \quad (7.52)$$

$$\simeq V^{sys} RT \sum_p \left[ C_p \ln \frac{C_p^{eq}}{C_p} + (C_p - C_p^{eq}) \right], \quad (7.53)$$

with  $p = R, C, P$  or  $W$ , and  $C_p^{eq}$  are the concentrations in equilibrium (see appendix 7.11). This exergy is always positive. The appendix 7.11 contains a derivation of this exergy expression, which is different from the original work by Mejer et al. Our alternative derivation even presents new interpretations of the different terms in (7.53), in terms of chemostat thermodynamical concepts such as the osmotic pressure.

The above expression requires correct knowledge of the equilibrium concentrations of consumer and predator. However, in real systems these concentrations are zero because a thermodynamic description breaks down. This complication is related with the fact that the biotic chemical potentials not necessarily exist. And as mentioned, there is also an arbitrariness in the reference thermodynamic equilibrium state of system and environments. This makes the exergy difficult to apply as a goal function candidate in far from equilibrium ecosystems. The above remarks indicate that of the two quantities, exergy and EP, only the latter can be determined without too much difficulties<sup>9</sup>.

#### A note on the exergy concept

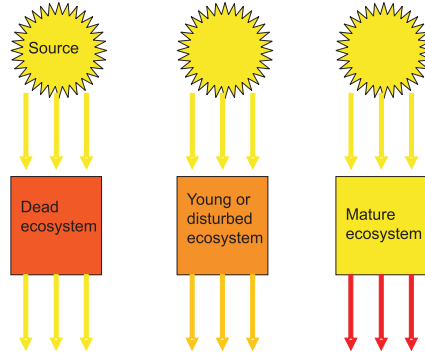


Figure 7.3: The exergy concept. Yellow color is high exergy, red color is low exergy. A dead system has low exergy content and low exergy destruction (dissipation), whereas a mature ecosystem is believed to have more or maximum exergy storage *and* exergy destruction.

One can say that the EP and the exergy are the two most important quantities in thermodynamic ecology. There are two competing schools. The 'MaxEx school' claims that in the ecosystem development there is a general trend towards a maximum exergy level (maximum storage), the 'MaxEP school' postulates that the trend is rather towards a maximum EP (exergy degradation

<sup>9</sup>That is one of the reasons why this thesis had its primary focus on the EP.

or dissipation). Others [202] conjectured that these two hypotheses might be mutually compatible in what is called the '*exergy concept*'. Fig. 7.3 gives the basics of the exergy concept (Muys, private communication). As ecosystems develop into more complex states, they might attain more ordered structures (with more exergy content), and these structures (the biota) might be more able to degrade *environmental* exergy. The *ecosystem* exergy is not degraded, as it might rather tend towards a maximum. The degradation of environmental exergy results in a production of entropy. Take the sun-earth system: A dead planet has low exergy and EP. But when life appears, there is 1) more order and therefore more exergy, and 2) these ordered organisms are more capable to increase the entropy of the emitted radiation. Roughly speaking, the exergy concept therefore states that the ecosystem exergy maximizes in order to maximally degrade the environmental exergy. However, the notions of environmental and ecosystem exergy, as well as the relation between environmental exergy degradation and EP needs more scrutiny. For the moment, the exergy concept remains a hypothesis, and its formulation uses words (exergy, order, exergy degradation,...) that are in need for refinement and clarity before they can be applied to ecosystems.

### Heat production

The heat production is also an important quantity in the study of ecosystem metabolism and allometry [187, 81]. Analogous to the chemical potentials (which are the partial molar Gibbs free energies) used in the entropy production, the heat production uses the partial molar enthalpies. They are defined as

$$h_p \equiv \left( \frac{\partial H}{\partial N_p} \right)_{p,T,N_{q \neq p}} \quad (7.54)$$

$$= -T^2 \frac{\partial(\mu_p/T)}{\partial T} \quad (7.55)$$

$$= \mu_p - T \left( \frac{\partial \mu_p}{\partial T} \right)_{p,T,N_{q \neq p}}. \quad (7.56)$$

For ideal fluids, and not taking into account the heat production from non-chemical processes (e.g. viscous dissipation of water flow), one can derive an expression for the heat production by taking the entropy production and changing in the affinities the chemical potentials with the molar enthalpies (see [88]):

$$\pi_{heat} = T\sigma(\mu_p \rightarrow h_p) \quad (7.57)$$

$$= - \sum_{\alpha} F_{\alpha} A_{\alpha}(\mu_p \rightarrow h_p) \quad (7.58)$$

$$= \sum_{\alpha} F_{\alpha} T^2 \frac{\partial \ln(\lambda_{\alpha}^{\leftarrow} / \lambda_{\alpha})}{\partial T}, \quad (7.59)$$

with  $F_{\alpha}$  the rate of the  $\alpha$ -th chemical reaction, and  $\lambda_{\alpha}^{\leftarrow}$  are the parameters in the  $\alpha$ -th reaction ( $\kappa_{AC}^{\leftarrow}, g_{\{CR,PC\}}^{\leftarrow}$  and  $d_{\{C,P\}}^{\leftarrow}$ ). So the heat production essentially depends on the temperature dependence of the reaction parameters. A priori, one can have both exothermic and endothermic reactions.

For the total heat production in the stationary state, the expression simplifies to

$$\pi_{heat,tot}^* = \alpha_R(C_R^0 - C_R^*)T^2 \frac{\partial \ln K_{eq}}{\partial T} \propto F_R^*, \quad (7.60)$$

which is essentially the total ecosystem metabolism at constant temperature.

### Other thermodynamic goal functions

The concepts energy and empower were introduced by Odum [141]. The **energy** is the free energy of one glucose molecule,  $\mu_R$ , (but perhaps one can also define it with the internal energy or partial molar enthalpy) times the number of glucose molecules needed to build the total biomass. The latter are given by the biomass concentrations divided by the yields.

$$Em \equiv \mu_R \left( \frac{C_C}{q_{CR}} + \frac{C_P}{q_{CR}q_{PC}} \right). \quad (7.61)$$

**Empower** can be defined as the free energy of one glucose molecule times the total flow from glucose to biomass (of only the consumer species)

$$Emp \equiv \mu_R q_{CR} q_{CR} C_C (C_R - C_W^0/K_{eq}). \quad (7.62)$$

One can postulate much more goal functions by taking products and ratios: The **benefit/cost** goal function [16] is a combination of 'optimal biomass structure', 'maximum benefits', 'minimal costs' and 'optimal information exchange' or 'performance'. Or putted more explicitly:

$$BC \equiv \frac{Ex.Asc}{Em.TST.NC}, \quad (7.63)$$

and in [10], the **energy/exergy ratio** was proposed as goal function.

These are the most important thermodynamic goal function proposals. It is now time to test them by using the solutions of our chemotropic ecosystem model.

## 7.6 Testing the goal function proposals

We have made a long list of possible goal functions (see table 7.1). The mathematical expressions are often very simple. With these expressions, one can test the proposals for all three definitions of a goal function.

### 7.6.1 Lyapunov goal function

The first definition requires a knowledge of the transient states. One can easily model this numerically, and see whether the proposal behaves as a Lyapunov goal function. We will leave a detailed study for future research. The general conclusion is that by some qualitative reasoning about the evolution of the transients, one can expect that none of the proposals appears to behave as a Lyapunov function for all relevant or theoretically possible parameter values and initial conditions. Only in some regions, some proposals might behave as Lyapunov functions.

living biomass	$B_{liv} \equiv C_C + C_P$
total biomass	$B_{tot} \equiv C_R + C_C + C_P$
exergy	$Ex \equiv \sum_p [C_p \ln(C_p^{eq}/C_p) + (C_p - C_p^{eq})]$
emergy	$Em \equiv \mu_R (C_C/q_{CR} + C_P/q_{CRq_{PC}})$
emergy/exergy	$Emex \equiv Em/Ex$
consumer residence time	$\tau_C = 1/(d_C + g_{PC}C_P)$
predator residence time	$\tau_P = 1/d_P$
average residence time	$\tau_{av} = \sum_{b=C,P} C_b \tau_b / \sum_{b=C,P} C_b$
consumer production	$P_C \equiv q_{CR}g_{CR}C_C(C_R - C_W^0/K_{eq})$
consumer specific production	$P_{C,spec} \equiv P_C/C_C$
system import	$SI \equiv \alpha_R(C_R^0 - C_R)$
system export	$SE \equiv F_{AC} + F_{cC} + F_{cP}$
biotic respiration	$R_B \equiv F_{cC} + F_{cP}$
respiration/biomass ratio	$RB \equiv R_B/B_{liv}$
cycling ratio	$Cyc \equiv \frac{\sum_{b=C,P} d_b C_b + \alpha_R C_R^0 + \kappa_{AC} C_W / K_{eq}}{\alpha_R C_R^0 + \kappa_{AC} C_W / K_{eq}}$
resilience	$Res \equiv -\max(\text{real}(\zeta(A)))$
reactivity	$Reac \equiv -\max\{\lambda(H(A))\}$
total system throughput	$TST \equiv \sum_{pq} F_{pq}$
network capacity	$NC \equiv \sum_{pq} \frac{F_{pq}}{\sum_{p'q'} F_{p'q'}} \ln \frac{F_{pq}}{\sum_{p'q'} F_{p'q'}}$
ascendency	$Asc \equiv \sum_{pq} F_{pq} \ln \left( \frac{F_{pq} \sum_{p'q'} F_{p'q'}}{\sum_r F_{pr} \sum_s F_{sq}} \right)$
consumer growth EP	$\sigma_{gCR} \equiv g_{CR}C_C(C_R - C_R^{eq}) \ln \frac{g_{CR}C_C^{1+q_{CR}}C_W^{1-q_{CR}}}{g_{CR}C_C C_R}$
consumer decay EP	$\sigma_{dC} \equiv d_C C_C \ln(d_C^- C_R / d_C C_C)$
predator growth EP	$\sigma_{gPC} \equiv g_{PC}C_P C_C \ln \frac{g_{PC}C_P^{1+q_{PC}}C_W^{1-q_{PC}}}{g_{PC}C_C C_P}$
predator decay EP	$\sigma_{dP} \equiv d_P C_P \ln(d_P^- C_R / d_P C_P)$
ecosystem metabolism EP	$\sigma_{EM} \equiv \sigma_{gCR} + \sigma_{dC} + \sigma_{gPC} + \sigma_{dP} + \kappa_{EM}(C_R - C_R^{eq}) \ln(C_R/C_R^{eq})$
total EP	$\sigma_{tot} \equiv \sigma_{EM} + \alpha_R(C_R^0 - C_R) \ln(C_R^0/C_R)$
heat production	$\pi_{heat} \equiv \sum_\alpha F_\alpha T^2 \partial \ln(\lambda_\alpha^- / \lambda_\alpha) / \partial T$
empower	$Emp \equiv \mu_R q_{CR} g_{CR} C_C (C_R - C_W^0/K_{eq})$
benefit/cost	$BC \equiv Ex.Asc/Em.TST.NC$

Table 7.1: The candidate goal functions. The first five are stocks, the others involve (inverse) rates.

The most famous - but ecologically unimportant - Lyapunov goal function is the exergy. It only works for systems whereby the reservoirs are in thermodynamic equilibrium ( $C_R^0 = C_W^0/K_{eq}$ ) and the system is near equilibrium with the reservoirs (which renders it useless for living ecosystems that have to operate far from equilibrium). The principle says that the exergy becomes minimal when the system is in thermodynamic equilibrium with its reservoirs. Hence, minus the exergy is the Lyapunov goal function. This is nothing but a reformulation of the second law of thermodynamics.

There is another famous and more general principle, which also works when the two environmental reservoirs are near equilibrium ( $C_R^0 \simeq C_W^0/K_{eq}$ ) and the system is also near equilibrium with the environments ( $C_R^0 \simeq C_R$ ). Again, no life is present, and hence it is less interesting from an ecological perspective. In this (near) equilibrium situation, the total EP has the property that it decreases ( $d\sigma_{tot}/dt < 0$ ), and it is minimal in the (near) equilibrium steady state. Hence, minus the total EP is a Lyapunov goal function for the (near) equilibrium system. This is a specific example of the famous Prigogine's minimum entropy production principle [88]. It is easy to see that this Lyapunov EP principle is no longer valid in the far from equilibrium regime. Therefore, Prigogine's MinEP is not applicable to living ecosystems, as incorrectly stated in e.g. [81].

### 7.6.2 Steady state goal function

The second definition requires a knowledge about evolution. If the consumer or the predator mutates, one only has to look at the evolutionary fitness, which is given by the two parameters  $\Phi_{\{C,P\}}$  (7.36) as defined before. All else being equal, the species with the highest fitness survives and the other competing species goes extinct. This gives a movement in parameter space for evolutionary timescales. This movement in parameter space is constrained by equations (7.84, 7.86, 7.87, 7.91). The movement is accompanied by a movement of the steady state in state space, and this property makes it easy to compare and test the goal function proposals of the initial and final steady states. Therefore, all goal function proposals which in the steady state only depend on these two quantities, might behave as evolutionary goal functions.

Of course, this principle is only relevant in the biotic states in ranges  $\mathcal{R}_2$  and  $\mathcal{R}_3$ . There is no simple correlation between the two parameters  $\Phi_{\{C,P\}}$  and the steady state values (7.30-7.35). This results in no simple correlation between the fitness and the goal functions, meaning that there are always parameter values and parameter changes such that the goal function proposal decreases under evolution.

We have already seen this situation for the total EP in section 6.3.3. Only (7.30) and (7.34) are clearly related with  $\Phi_{\{C,P\}}^{-1}$ . In other words, the total EP is a steady state goal function in range  $\mathcal{R}_2$ , as it increases under consumer evolution. But in range  $\mathcal{R}_3$  the situation gets more troublesome, as the total EP decreases under predator evolution and yet increases under consumer evolution.

### 7.6.3 Non-variational goal function

The third definition compares the different steady states of the (non-evolutionary) ecosystem population dynamics (7.19-7.21). One simply has to evaluate the goal function proposal in all possible steady states, and see whether it is correlated

with the stability (7.46), as shown in fig 7.2. If the most stable steady state has the highest value for the GF proposal (for all relevant values of the parameters), then the proposal is a good goal function.

The major result is that none of the above goal function proposals satisfy this property in all relevant parameter regimes (especially in the third regime of the driving force parameter  $\Delta$ ).

We have already seen that the total EP (and the situation for the ecosystem metabolic EP is similar) does not obey the non-variational MaxEP hypothesis. Also the exergy is generally not a good goal function for none of the three regimes. Since the exergy expression explicitly depends on the reference chemical potentials  $\mu_p^r$ , and since the latter can a priori be arbitrary (except for the constraints (7.87), one can easily show that there are a priori possible theoretical values of these chemical potentials such that the exergy is invalid as a goal function. However, as Jørgensen pointed out ([81] p.173), in realistic ecosystems the chemical potentials might have values such that the non-variational property becomes valid in all three ranges. However, his calculations of the biotic chemical potentials remains doubtful.

We are not going to write down the explicit parameter criteria for a specific goal function proposals to be valid in specified ranges. By playing around with the parameters, the general conclusion is that none of the proposals are really satisfying in all relevant parameter regimes (all three ranges).

## 7.7 Efficiency measures

Efficiencies are very important in the study of energy processing in biological activity. Efficiency measures are dimensionless numbers between zero and one. One can construct a lot of them, but not all of them will be ecologically or physically important or meaningful. Also the efficiency measures can serve as possible goal functions. In this section we will again define rigorously some efficiency measures, and they can also be grouped into kinetic and thermodynamic ones. In the next section we will try to find relationships between all the measures. For example, it is widely believed that the efficiency of biological activity increases under evolution.

### 7.7.1 Kinetic efficiencies

The kinetic efficiencies only depend on the variables and the kinetic parameters. We will list the following flow efficiencies.

- The **ecosystem flow efficiency**

$$\eta_{FE} \equiv \frac{F_{aC}}{F_{gCR} + F_{AC}}. \quad (7.64)$$

- The **consumer and predator flow efficiency** (yield)

$$\eta_{FC} \equiv \frac{F_{aC}}{F_{gCR}} = q_{CR}, \quad (7.65)$$

$$\eta_{FP} \equiv q_{PC}. \quad (7.66)$$

- The **cycling efficiency**

$$\eta_{cyc} \equiv \frac{\sum_{b=C,P} d_b C_b}{\sum_{b'=C,P} d_{b'} C_{b'} + \alpha_R C_R^0 + \kappa_{AC} C_W / K_{eq}} = 1 - \frac{1}{C_{yc}}. \quad (7.67)$$

- The **resource conversion efficiency**

$$\eta_{RC} \equiv \frac{F_{SE}^*}{F_{SE,max}^*} = \frac{F_{AC}^* + F_{cC}^* + F_{cP}^*}{\alpha_R (C_R^0 - C_W^0 / K_{eq})}, \quad (7.68)$$

with  $F_{SE,max}^*$  the maximum system export in the steady state. This maximum is reached when the resource conversion is maximal, such that  $C_R^* \approx C_W^0 / K_{eq}$ . The quantity  $\eta_{RC}$  is always less than unity (and hence an efficiency) when the system is in a steady state. In the steady state, the resource uptake, the resource conversion and the system export are all equal.

### 7.7.2 Thermodynamic efficiencies

The thermodynamic efficiencies again involve energy measures, like chemical potentials.

- The **total chemical Carnot efficiency**

$$\eta_{Car} \equiv \frac{\mu_R^0 - \mu_W^0}{\mu_R^0}, \quad (7.69)$$

as the chemical analogue for Carnot efficiency of a heat engine<sup>10</sup>.

- The **ecosystem chemical Carnot efficiency**

$$\eta_{Car,E} \equiv \frac{\mu_R - \mu_W}{\mu_R}. \quad (7.70)$$

- The **first law thermodynamic consumer efficiency**

$$\eta_{1L,C} \equiv \frac{F_{aC} A_{aC}}{\alpha_R C_R^0 \mu_R^0} = \frac{\text{anabolic work rate}}{\text{total energy input}}, \quad (7.71)$$

- The **second law thermodynamic consumer efficiency**

$$\eta_{2L,C} \equiv \frac{F_{aC} A_{aC}}{T \sigma_{tot}} = \frac{\text{anabolic work rate}}{\text{maximum work rate}}. \quad (7.72)$$

- The **anabolic-catabolic (A-C) coupling consumer and predator efficiency** [205]

$$\eta_{ac,C} \equiv \frac{F_{aC} A_{aC}}{-F_{cC} A_{cC}} = \frac{\text{anabolic work rate}}{\text{catabolic work rate}}, \quad (7.73)$$

$$\eta_{ac,P} \equiv \frac{F_{aP} A_{aP}}{-F_{cP} A_{cP}}. \quad (7.74)$$

<sup>10</sup>The Carnot efficiency of a heat engine operating between high temperature  $T_H$  and low temperature  $T_L$  is given by  $\eta = (T_H - T_L)/T_H$ . Translating the temperatures as  $T \rightarrow \mu/T$  (i.e. translating thermodynamic intensive quantities) gives the Carnot efficiency for a chemical engine.

- The **consumer and predator energetic efficiency**

$$\eta_{EC} \equiv \frac{F_{aC}\mu_C}{F_{gCR}\mu_R} \quad (7.75)$$

$$\eta_{EP} \equiv \frac{F_{aP}\mu_P}{F_{gPC}\mu_C} \quad (7.76)$$

- The **ecological efficiency** [39, 155]

$$\eta_E \equiv \frac{F_{aP}^*\mu_P^*}{F_{gCR}^*\mu_R^*} \quad (7.77)$$

Note that the latter efficiencies depend on the biotic chemical potentials which are difficult to measure.

The first law thermodynamic efficiency relates the useful work output to the total energy input. This work output is taken here as the growth of biomass. Remark that due to biomass decay or turnover (a kind of friction term), the work output is eventually dissipated. The latter biomass turnover (work loss) is not taken up in the first law efficiency, because otherwise this efficiency would be zero.

All efficiencies are by definition numbers between 0 and 1. E.g. the coupling efficiency  $\eta_{ac,C} \leq 1$  is derived from the positivity of the growth EP:

$$0 \leq T\sigma_{gC} = -F_{gCR}A_{gCR} \quad (7.78)$$

$$= -F_{aC}A_{aC} - F_{cC}A_{cC}. \quad (7.79)$$

## 7.8 Searching for relationships between the measures

With all the above definitions for parametric, goal function and efficiency measures, one can look for relations between them. The amount of possible relations is very high<sup>11</sup>. Here we will only make comments on some possible relations. We will especially highlight an important discussion relating evolution, (thermodynamic) efficiency and entropy production.

First, there are some (trivial) relations and constraints between efficiency measures, e.g.

$$\eta_{Car,E} \leq \eta_{Car}, \quad (7.80)$$

$$\eta_{FE} \leq \eta_{FC}, \quad (7.81)$$

$$\eta_{1L,C} = \eta_{Car}\eta_{2L,C}. \quad (7.82)$$

A more interesting natural possibility is the existence of correlations between efficiency measures and evolutionary fitness, as can be seen in e.g. the statement by Lotka [100]: "Species which utilize portions of the flow of available energy most efficiently (all other things being equal) for their growth and existence will increase their population and, therefore, the flow of energy through the system

<sup>11</sup>If there are  $n$  quantities, the number of possibilities scale as  $n^2/2$ . The number of measures we encountered is more than 40, which gives more than 1000 possible relations.

will increase.” This expression related fitness, biomass, total system throughput and (some) efficiency measure. Statements like this one are rather frequent in the thermodynamic ecology literature. More generally, one can ask the question: Are organisms or ecosystems evolving towards a more efficient behavior? This is equivalent with asking whether the efficiencies are steady state goal functions. In order to study this question, one has to look at the behavior of the steady states when the fitness is changed. The fitness might change under combinations of changes in growth rate, decay rate and yield. If one or more of these parameters changes, also other parameters have to change in order to satisfy the constraints (7.84-7.91).

The general conclusion is that there are no clear correlations between fitness and efficiency for all relevant (and theoretically possible) parameter values. Hence, the efficiencies are not general steady state goal functions. Only the system Carnot efficiency  $\eta_{Car,E}$  in regime  $\mathcal{R}_2$  depends only on  $\Phi_C$ . When the consumer fitness increases,  $\eta_{Car,E}$  decreases. The reason why this efficiency decreases is that when the consumers become fitter, they are more able to deplete the resource, and therefore the ecosystem resource concentration  $C_R^*$  will lower. This means that the internal distance from equilibrium, as measured by  $C_R^* - C_R^{eq}$  decreases, making the ‘chemical Carnot engine’ that operates inside the system less efficient. This also means that there is an increasing amount of the work input dissipated, because the mixing EP associated with the inflow  $F_R = \alpha_R(C_R^0 - C_R^*)$  increases when  $C_R^*$  decreases.

If we look at the yield efficiency  $q_{CR}$ , one might expect that this is positively correlated with the consumer fitness. However, it is possible that the evolution of the consumer has to deal with a trade-off between yield and growth: The fitness might increase when the growth increases, but at the same time the yield efficiency might decrease.

If one only changes the growth rate, the death rate or the yield parameters separately (no trade-offs between these parameters), and all else equal, then one can find correlations for most parameter values. For example, when only the growth rate increases in regime  $\mathcal{R}_2$ , then one can see that this change is positively correlated with  $\eta_{FE}$ ,  $\eta_{1L,C}$ ,  $\eta_{2L,C}$  and  $\eta_{ac,C}$ .

A final interesting discussion is the question whether the relation between evolutionary fitness, efficiency and EP holds. This is stated in e.g. [85] as “[...] this puts a preferred direction on natural selection for those organisms which increase degradation of free energy, or equivalently, entropy production”, and also in [99] or [94]: “The evolution of efficient metabolisms is equivalent to the evolution of larger EP. This trend is presumably due to the fact that life-forms that can extract more work (and therefore produce more entropy), survive preferentially”. One has to make these statements more precise as to what definitions for EP and efficiency were used. The general conclusion is again negative: There are no clear correlations between the three measures (fitness, efficiency and EP) for all relevant parameter regimes.

## 7.9 Conclusion

In order to study the general behavior, evolution, stability or steady states of an ecological system, one can try to look at goal function and efficiency measures.

With a simple chemotrophic resource-consumer-predator ecosystem model

we were able to quantitatively define a lot of goal functions and efficiencies. We could classify them into kinetic and thermodynamic measures. The thermodynamic measures are highly used in physics, and one is tempted to look at them from an ecological perspective. The biggest problem regarding this thermodynamic point of view is that the chemical potentials of the biota are difficult to measure or to calculate. This remains one of the biggest challenges in thermodynamic ecology.

With the (thermodynamically consistent) mathematical expressions and definitions, we can look at the behavior under ecological or evolutionary dynamics and try to find correlations between these measures. In this research, no general positive results were obtained: Only a few non-trivial relations were found and none of the proposed goal function measures satisfy any of the proposed goal function definitions in all relevant parameter regimes. We should keep in mind that the model studied was highly simplified and purely theoretical.

The pessimistic attitude might say that if it is so easy to find counter-examples for goal functions and other correlations, then one should be very sceptic for more complex systems. The optimistic attitude on the other hand claims that complexity might 'save' one or more goal functions, and further research is needed<sup>12</sup>.

Nevertheless, we were able to demonstrate the correctness of some measures in specific parameter regimes. Some goal functions (e.g. the total EP) are valid in resource-consumer ecosystems, but they become invalid when a predator is included in the system. As humans have a predatory impact on nature, one might perhaps use these results in order to search for a measure for the ecological impact of humans.

## 7.10 Appendix: Parameter constraints and model simplifications

In this appendix we will explain some simplifications for the reaction rates. In order to justify these simplifications, we first need to derive some constraints on the parameters, which are imposed by thermodynamic consistency.

### Parameter constraints

First of all, all parameters  $\kappa_{AC}^{(\leftarrow)}$ ,  $g_{(CR,PC)}^{(\leftarrow)}$ ,  $q_{(CR,PC)}$  and  $d_{(C,P)}^{(\leftarrow)}$  should be positive. Secondly, we have the requirement that the yields  $q_{CR} < 1$  and  $q_{PC} < 1$ . Furthermore, one can easily see the thermodynamic closure relation of the affinities (the law of Hess [88])

$$A_{gCR} = (1 - q_{CR})A_{AC} - q_{CR}A_{dC}, \quad (7.83)$$

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<sup>12</sup>I have studied the EP in a lot of other models which are not taken up in this thesis: models with multiple essential resources [67], nutrient cycling [46], top predators, evolutionary feedback [2], whole-cell modeling formulations [124], time-delayed chemostats [17], fluctuations [137], other growth kinetics (functional responses like e.g. Michaelis-Menten), gradostats, inhibitors, variable-yield, size structure,... [185]. In all these models it was all too easy to find (allowed) parameter values such that the EP was not a goal function.

and this gives the following constraint on the parameters:

$$1 = \frac{g_{CR}}{g_{CR}^{\leftarrow}} \left( \frac{\kappa_{AC}^{\leftarrow}}{\kappa_{AC}} \right)^{1-q_{CR}} \left( \frac{d_C}{d_C^{\leftarrow}} \right)^{q_{CR}}. \quad (7.84)$$

There is a same kind of constraint for the predator:

$$A_{gPC} = (1 - q_{PC})A_{AC} - q_{PC}A_{dP} + A_{dC}, \quad (7.85)$$

$$1 = \frac{g_{PC}}{g_{PC}^{\leftarrow}} \left( \frac{\kappa_{AC}^{\leftarrow}}{\kappa_{AC}} \right)^{1-q_{PC}} \left( \frac{d_P}{d_P^{\leftarrow}} \right)^{q_{PC}} \frac{d_C^{\leftarrow}}{d_C} \quad (7.86)$$

These parameters are also related to the reference chemical potentials  $\mu_p^r$  as follows:

$$\mu_R^r - \mu_W^r = RT \ln \frac{\kappa_{AC}}{\kappa_{AC}^{\leftarrow}}, \quad (7.87)$$

$$q_{CR}\mu_C^r + (1 - q_{CR})\mu_W^r - \mu_R^r = RT \ln \frac{g_{CR}^{\leftarrow}}{g_{CR}}, \quad (7.88)$$

$$\mu_R^r - \mu_C^r = RT \ln \frac{d_C^{\leftarrow}}{d_C}, \quad (7.89)$$

$$q_{PC}\mu_P^r + (1 - q_{PC})\mu_W^r - \mu_C^r = RT \ln \frac{g_{PC}^{\leftarrow}}{g_{PC}}, \quad (7.90)$$

$$\mu_R^r - \mu_P^r = RT \ln \frac{d_P^{\leftarrow}}{d_P}. \quad (7.91)$$

These constraints are necessary and sufficient in order to understand the thermodynamic consistency of the simplifications we are going to perform.

### Model simplifications

Let us list the simplification of the fluxes and rates.

- We will restrict to a constant inflow of glucose, at rate  $\alpha_R C_R^0$ . There's also an outflow of glucose back to the external reservoir at rate  $-\alpha_R C_R$ , so the net glucose exchange rate is  $\alpha_R(C_R^0 - C_R)$ .
- For the net  $CO_2$  waste exchange rate, we will take the same expression  $\alpha_W(C_W^0 - C_W)$ .
- The specific waste exchange rate  $\alpha_W$  will be taken very high (infinite), such that we can approximate  $C_W \simeq C_W^0$ , and hence we have only three variables  $C_R$ ,  $C_C$  and  $C_P$  left.
- With the help of the (thermodynamic) parameter constraint (7.84), the consumer growth rate can be written as

$$F_{gC} = g_{CR}C_C \left( C_R - \left( \frac{d_C C_C}{d_C^{\leftarrow} C_R^{eq}} \right)^{q_{CR}} C_R^{eq} \right) \quad (7.92)$$

$$\leq g_{CR}C_C(C_R - C_R^{eq}). \quad (7.93)$$

When  $q_{CR} \ll 1$ , the above inequality approaches the equality. We will approximate the growth rate by the latter equality. This means that the growth becomes thermodynamically impossible when the resource concentration is at the thermodynamic equilibrium value.

- Also for the predator growth rate we have

$$F_{gP} = g_{PC} C_P \left( C_C - \frac{d_C^-}{d_C} \left( \frac{d_P C_P}{d_P^- C_R^{eq}} \right)^{q_{PC}} C_R^{eq} \right) \quad (7.94)$$

$$\leq g_{PC} C_P C_C. \quad (7.95)$$

Also here we will take the equality as an approximation, which is valid when  $q_{PC} \ll 1$  and  $d_C^- \ll d_C$ .

- In the decay rates, the backward rates  $F_{d,\leftarrow} \approx 0$  because  $d_{C,P}^-$  are assumed to be very small. However, in the affinity expressions, the latter parameters can not be neglected because they have a logarithmic dependence.

## 7.11 Appendix: Derivation of the exergy function

In order to derive the exergy, one could decouple the resource reservoir from the system ( $\alpha_R \rightarrow 0$ ). This means that the waste reservoir sets the reference. Let us calculate the exergy as the total Gibbs free energy difference at constant temperature and pressure. Let us write  $C_p = N_p/V^{sys}$  as the concentrations of the solutes in the system. The solutes are the carbonic compartments resource, consumer biomass, predator biomass, and waste. The system solvent is water (including the oxygen), at high concentration  $C_S$ . We make the important approximation that the carbonic compounds are in a dilute solution, which means that  $C_p \ll C_S$ . The total concentration  $\sum_p C_p + C_S \approx C_S$  is approximately constant. The chemical potential for the solvent is [88]

$$\mu_S(p_S, T) = \mu(T) + p_S/C_S, \quad (7.96)$$

with  $p_S$  the pressure generated by the solvent.

Starting from the initial (superscript  $i$ ) solute concentrations  $C_p^i$ , the system relaxes to the equilibrium  $C_p^{eq}$ . These equilibrium values are

$$C_R^{eq} = \frac{C_W^0}{K_{eq}}, \quad (7.97)$$

$$C_C^{eq} = \frac{d_C^- C_W^0}{d_C K_{eq}}, \quad (7.98)$$

$$C_P^{eq} = \frac{d_P^- C_W^0}{d_P K_{eq}}, \quad (7.99)$$

$$C_W^{eq} = C_W^0 = C_W^i, \quad (7.100)$$

where we have applied the constancy of the waste concentration due to the infinite exchange rate with the large waste environment at constant concentration. The equilibrium values for biomass are very small, but they can not be neglected in logarithm terms as we will see.

During this relaxation process to equilibrium, there is solute particle exchange with the environment, such that the number of particles in the reservoir changes with  $\Delta N^0 = -\Delta N = -\Delta(\sum_p N_p)$ , whereby  $\Delta N = N^{eq} - N^i$  equals

the difference between the final equilibrium and the initial value. This means that there is a change in environmental free energy equal to

$$\Delta G^0 = -\mu_W^0 \Delta N, \quad (7.101)$$

with  $\mu_W^0$  constant. For the total free energy change of the system, we start with the following: The free energy change of the solutes equals

$$\Delta G_{sol} = \Delta \left( \sum_p \mu_p N_p \right). \quad (7.102)$$

Adding  $\Delta G^0 + \Delta G_{sol}$ , we get

$$\Delta G^0 + \Delta G_{sol} = \Delta \sum_p (\mu_p - \mu_W^0) N_p \quad (7.103)$$

$$= \sum_p (\mu_p^{eq} - \mu_W^{eq}) N_p^{eq} - \sum_p (\mu_p^i - \mu_W^0) N_p^i \quad (7.104)$$

$$= - \sum_p (\mu_p^i - \mu_W^0) N_p^i \quad (7.105)$$

$$= - \sum_p RT \left( \ln \frac{C_p^i}{C_p^{eq}} \right) N_p^i, \quad (7.106)$$

where we have used the equilibrium condition  $\mu_p^{eq} = \mu_W^{eq} = \mu_W^0$ .

However, there is also a free energy change coming from the solvent which is related with a change in osmotic pressure. The solutes create an osmotic pressure which might be approximated by the ideal gas equation of state [88]:  $\pi = \sum_p \pi_p = \sum_p C_p RT$ . With (7.96), the solvent chemical potential equals

$$\mu_S(p_S, T) = \mu_S(p_S + \pi, T) - \pi / C_S. \quad (7.107)$$

The system is in contact with an environment at constant pressure  $p^0$  and this equals  $p_S + \pi$ . With (7.107) and the constancy of  $p_S + \pi$ , the change in solvent chemical potential is  $\Delta \mu_S = -\Delta \pi / C_S$ . This gives a change in free energy from the solvent:

$$\Delta G_{solv} = N_S \Delta \mu_S \quad (7.108)$$

$$= -V^{sys} \Delta \pi \quad (7.109)$$

$$= -V^{sys} \Delta RT \sum_p C_p \quad (7.110)$$

$$= -RT \sum_p (N_p^{eq} - N_p^i). \quad (7.111)$$

Adding  $\Delta G^0 + \Delta G_{sol} + \Delta G_{solv}$  gives

$$Ex \equiv \Delta G_{tot} = - \sum_p RT \left( \ln \frac{C_p^i}{C_p^{eq}} \right) N_p^i - RT \sum_p (N_p^{eq} - N_p^i) \quad (7.112)$$

$$= V^{sys} RT \sum_p \left[ C_p^i \ln \frac{C_p^{eq}}{C_p^i} + (C_p^i - C_p^{eq}) \right]. \quad (7.113)$$

This is exactly the same equation that Mejer and Jørgensen derived [81, 116]. However, here we have given it a concrete physical meaning, denoting e.g. terms coming from osmotic pressure. Note that this total Gibbs free energy change is always negative, and it only depends on the solute concentrations, not on the solvent.

## Chapter 8

# Ecosystems and dissipative structures: Does life increase the entropy production?

### Abstract<sup>1</sup>

It is hypothesized that living organisms are dissipative structures. However, the definition of a dissipative structure is often quite vague, making it difficult to test this hypothesis. Here we will formulate some testable statements related to the study of the dissipative character of ecosystems. This leads us to a simple yet non-trivial definition of a dissipative structure, based on two criteria: a non-trivial bifurcation and an entropy production (EP) enhancement. The latter criterium is related with the work by Ulanowicz and Hannon [199]. To see whether biological structures are dissipative structures, we will focus at the population level, by presenting phototrophic and chemotrophic ecosystem models and calculating the EP of these two systems. It is shown that some parameter values can result into 'infra dissipative' behavior, which means that the biotic state has a lower EP than the corresponding abiotic state. This allows us to give comments on the hypothesis by Ulanowicz and Hannon, and on the possibility for organisms to be dissipative structures.

### 8.1 Introduction

Dissipation is the production of entropy, which occurs by irreversible processes in non-equilibrium systems. In this sense, biological and ecological systems are examples of such non-equilibrium, dissipative systems, because biological processes naturally produce entropy. But these systems are not only dissipative, but also self-organizing. In dissipative and self-organizing systems, ordered structures and spatial or temporal patterns might spontaneously appear. This lead Prigogine and co-workers [65, 88, 134] to the formulation of so called 'dissipative

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<sup>1</sup>This chapter is based on an article in preparation.

structures'. Biological structures, from the subcellular level (autocatalytic chemical reaction cycles) to the macro-ecological level (particular spatial patterns in landscapes) are often presented as examples of dissipative structures [135].

However, it is difficult to find in the literature a rigorous and formal definition of a dissipative structure such that one can test the hypothesis that living beings are indeed dissipative structures. Simply stating that life and other regular patterns that appear in the world are dissipative structures because they are structured and they dissipate energy or matter, is too trivial to be useful for predictions. Any non-equilibrium system dissipates (produces entropy) according to the second law. Take for example the letters on this page. These letters are clearly structured, and as light is absorbed and emitted, this page also produces entropy. However, the letters did not spontaneously arise due to a self-organizing process. These letters will not be called dissipative structures.

One can try something less trivial, e.g. "quantifying the ordered complexity" and "measuring the degree of self-organization" of those structures (using e.g. information theory [55] or extremal principles [62]), but that remains a very difficult and confusing task. The above two statements were placed between quotation marks because it is not clear when the problem is solved. How do we know that we have really quantified the complexity? As these statements are too vague, are there simpler and yet non-trivial characteristics or criteria to define dissipative structures?

In the first section, we will present a definition of a dissipative structure, which contains two criteria. One of these criteria, the increase of entropy production (EP) by the dissipative structures, is related to the work by Ulanowicz and Hannon [199]. Ulanowicz and Hannon presented some intuitive arguments for the hypothesis that, for the same system with the same boundary conditions, the ordered, living state (if life can persist) has a higher entropy production than the dead state. Intuitively, a living state is more 'active', and its irreversibility is therefore higher because there are more pathways to dissipate energy.

Presenting a definition is one thing, but the major part of our study focuses on specific ecosystem models to see whether the organisms in these systems really are dissipative structures and whether the proposal by Ulanowicz and Hannon is correct. Studying these models allows us to answer more quantitatively questions like "Are living processes 'more irreversible' than abiotic processes?" or "Does life increase the production of energetic disorder in the universe?"

Our first model will be a phototrophic ecosystem. It can be considered as a simplified, 'zero dimensional' Gaia model [203], with biological feedback on the albedo factor. Some general thermodynamic aspects of such feedback mechanisms were studied by Kleidon [85]. We will deepen this understanding of phototrophic ecosystems by explicitly solving our specific model and by calculating the EP to see how it behaves under different circumstances. Our second model consists of a chemotrophic ecosystem. By analogy with the phototrophic system, a biological feedback mechanism is included. This might simulate bioturbation and bio-irrigation in ocean sediment ecosystems [118]), and it allows us to study thermodynamic consequences of such feedbacks.

## 8.2 A definition of dissipative structures

A dissipative system is an open system that is driven out of thermodynamic equilibrium because it is coupled with a non-equilibrium environment that typically consists out of different reservoirs (e.g. heat baths) in mutual disequilibrium. Due to this coupling, energy and/or matter can flow through the system. This throughflow is the consequence of an external driving force, an applied thermodynamic gradient that the environment imposes on the system. There are some particular dissipative systems far enough from equilibrium, where non-linear effects become important, and macroscopic system variables become subjected to (positive) feedback mechanisms, which results in some 'self-organizing' behavior. These systems are therefore called 'self-organizing dissipative systems'.

This 'self-organization' is related with the intriguing behavior of (apparently) spontaneous fluctuations. At or very close to thermodynamic equilibrium, such fluctuations die out at relatively short timescales, because these fluctuations typically decrease the system entropy. However, far from equilibrium, due to the feedback mechanisms, some fluctuations can evade this rapid decay to equilibrium, and persist for relatively long times. Even more remarkably, initially small or improbable fluctuations can become enlarged by positive feedback effects. The persistent structures or patterns that might arise from the fluctuations are breaking some spatial or temporal symmetries of the equilibrium system. These structures maintain themselves by taking up low entropic energy/matter from the environment and discharging high entropic energy/matter to the environment. In other words, the maintenance of these structures is accompanied with dissipation of energy/matter. Therefore, these structures are termed dissipative structures<sup>2</sup>. When the environmental reservoirs are finite, the applied gradients will (slowly) decrease due to the dissipation. Therefore, the dissipative structures will contribute to the degradation of these gradients.

It is tempting to apply the above formulation to biological systems. Lotka [99] conjectured a higher energy throughflow through the ecosystem because organisms increase the energy capture from the environment. Boltzmann and Schrödinger [182] pointed out that life lives on low entropic energy/matter, Morowitz [125] discussed some consequences of a system with a continuous throughflow of energy/matter, Prigogine et al. [88, 134] discussed self-organizing spatial and temporal patterns abundant in biology and ecology, and Schneider et al. [178, 179, 181] conjectured an analogy between ecological systems and other 'gradient degrading' physical systems, such as Rayleigh-Bénard cells (see also Atkins [8]). The work by Schneider et al. might guide us towards a definition of dissipative structures.

Fig. 8.1 shows the total EP  $\sigma^*$  in the steady states (denoted with a superscript \*) for the Rayleigh-Bénard convective fluid system, a horizontal viscous fluid layer which is heated from below. This fluid system shows an intriguing behavior: convection cells form an ordered pattern that arises after reaching a critical threshold of the vertical temperature gradient  $\Delta$  (the temperature

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<sup>2</sup>Perhaps the name 'dissipative structure' is not well chosen, because not only maintenance, but basically all irreversible processes dissipate energy or matter. Consider again the letters on this page. Although they dissipate energy, they are not considered dissipative structures because there is no 'self-organization' and maintenance. As all non-equilibrium systems, this page is a dissipative system (it produces entropy), but it does not have dissipative structures, even though there are structures on it.

difference between lower and upper boundary). Therefore, this fluid system is considered as a prime example of a self-organizing dissipative system with the convection cells as the dissipative structures. Plotting the EP in function of  $\Delta$ , one can see that the thermal conduction states are located on the '*thermodynamic branch*', so called because it contains thermodynamic equilibrium at zero gradient. These steady states are stable when  $\Delta < \Delta_c$ . But above the critical threshold, an exchange of stability occurs: the new stable steady states are the convection states, and they form the '*structure branch*'. Hence,  $\Delta_c$  is a transcritical bifurcation point.

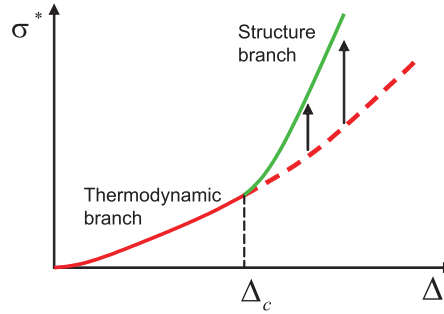


Figure 8.1: The EP in function of the applied thermodynamic gradient  $\Delta$  in a self-organizing dissipative system with dissipative structures. Red is the thermodynamic branch, green is the structure branch. Solid curves represent the stable states, dashed curves are the unstable states. At  $\Delta_c$ , there is an exchange of stability.

With the above discussion, we can more rigorously formulate a definition of a dissipative structure. Fig. 8.1 will serve as a fingerprint for dissipative structures, from which we can derive two testable properties: a non-trivial bifurcation and an EP increase. To make it more accurate, we first have to specify a non-ambiguous measure for the overall distance from equilibrium: the applied thermodynamic gradient  $\Delta$ . (We will not deal with systems having more than one applied gradient.) This is only possible when the environment has two reservoirs in internal equilibrium, and  $\Delta$  is typically the difference of an intensive thermodynamic quantity (e.g. temperature) of the two reservoirs. This gradient serves as a bifurcation parameter, i.e. we will look at the steady states, and study their behavior and asymptotic stability as the bifurcation parameter changes. For more general attractor states ((pseudo-)periodic or chaotic states), one can take time averages. Our definition now consists of two criteria:

*A non-trivial bifurcation.* As dissipative structures cannot survive arbitrarily close to equilibrium, there should be a minimum distance from equilibrium, a non-trivial bifurcation point  $\Delta_c$ , below which the structures can not persist.

*An increased EP.* As the structures are dissipating energy to maintain themselves, they should have a positive EP. This is always satisfied by the second law, so it is more interesting to look at the EP relative to the thermodynamic branch state, i.e. the steady state corresponding with the same applied gradient value, but without any persisting macroscopic dissipative structures. The dissipative structure should have *ultra dissipative* behavior, i.e. the stable dissipative structure state should have a higher EP than its corresponding unstable state at the

thermodynamic branch. When the stable structure state has a lower EP, the system is said to be in an *infra dissipative state*, and the associated structures may be termed 'anti-dissipative' rather than 'dissipative' structures.

### 8.3 Biological structures as dissipative structures?

The above two criteria, the increased EP and the non-trivial bifurcation, reflect the two words 'dissipative' and 'structure' respectively. The bifurcation indicates a symmetry breaking, a non-equilibrium phase transition from a homogeneous (translation invariant) to a structured state that breaks the spatial or temporal translation symmetry. Note that our definition does not imply that we have to specify the structures: No mention was made of measuring temporal or spatial properties of the patterns. We can take time-averages such that cyclical behavior becomes invisible, or we can take a homogenized or spatially averaged description of the system such that spatial patterns become invisible. In this way, we escape the problem how to quantify the 'ordered complexity': We only have to look at the external gradient and the global, time-averaged EP of the system.

The second criterium, the EP enhancement, is identical to the hypothesis by Ulanowicz and Hannon [199] for biological systems. They stated that "the second law, in combination with the observed increase in order of living systems, implies that life increases the amount of entropy generated in the universe," and "positive feedback, a fundamental element of the life process, serves to augment the total dissipation by a living system."

Coming back to our example of the letters on this page, it is clear that our definition exclude these letters from being dissipative structures. The gradient might e.g. measure the difference in wavelength of the absorbed and emitted radiation. Placing this page in an isolated black box, its radiation will attain equilibrium, but the structures are still there. There is no bifurcation.

But how to apply our definition to biological structures, or more generally to observed patterns that are often mentioned in the context of dissipative structures, such as wavy patterns (e.g. sand dunes), chemical oscillations [134], Turing patterns in reaction-diffusion systems, living cells, organisms, populations, predator-prey oscillations [8] or self-organized patchiness in landscapes [167]? It seems that there are some practical problems related with our definition: The gradient should be well defined, and we have to be able to calculate the total (time-averaged) EP for the states at the thermodynamic and the structure branches. More fundamentally, we have to be precise about the distinction between a dissipative structure, the system of dissipative structures and its environment. Also the scale of the structures and the systems are important in biology. What is the environment of a population, of a multi-cellular organism or of a single cell in this organism? And what if the environment is not simply given by two large reservoirs in internal equilibrium?

We will not go into all these questions, but in this study we will look at one specific level, the population of organisms. In the next two sections, we will look at theoretical phototrophic and chemotrophic ecosystem models with well defined gradients, and examine whether they have non-trivial bifurcation

points and are in *infra* or *ultra* dissipative states. As our definition for dissipative structures does not involve a characterization of the spatial patterns (e.g. the size of the organisms), it will suffice to take a spatial average of the system variables. Even if we know that individual organisms are structured, they can not be described explicitly as a consequence of our homogenization. This simplification results in two variables, an abiotic and a biotic one, and as is usually done in theoretical ecology, we will postulate dynamical equations based on intuition and known laws. The two dynamical equations for the two variables will be rich enough to describe a non-trivial bifurcation behavior.

After solving the dynamics for the steady states, consistent quantitative expressions for the steady state EP are written down, based on the formalism of local-equilibrium thermodynamics. These EP expressions are now functions of the parameters of the dynamical equations. The important result is that there are parameter values for which the biotic state is *infra* dissipative. There are no laws known that exclude these values for the parameters. Therefore we can conclude that living organisms are not always dissipative structures, or there should be yet unknown restrictions on the parameter values to save the *ultra* dissipative behavior.

## 8.4 The phototrophic ecosystem

### 8.4.1 The set-up

Phototrophic ecosystems are based on radiation as the primary energy source (see [156] for a thorough discussion on the thermodynamics of radiation). The ecosystem (e.g. the earth covered with vegetation, or a Daisyworld ecosystem [203]) is thermodynamically coupled with a non equilibrium environment, consisting of a black body radiation source (e.g. the sun) at high temperature  $T_H^0$ , and a (black body) background (e.g. interstellar space) at a negligibly small temperature  $T_L^0 \approx 0$  (the superscript 0 denotes an environmental constant). The ecosystem contains abiotic elements (e.g. bare soil) and biota (e.g. plants) that cover a fraction  $B \leq 1$  of the ecosystem. This fraction (e.g. the vegetation cover for a terrestrial ecosystem) is normalized such that when  $B = 1$ , the whole ecosystem is occupied by biota and all abiotic elements are completely covered (shaded). We assume fast heat exchange between abiotic and biotic elements in the ecosystem, such that both have the same temperature, the variable ecosystem temperature  $T_E$ .<sup>3</sup>

### 8.4.2 The dynamics

The model description has two variables: an abiotic temperature  $T_E(t)$  and a biotic fraction  $B(t)$ . Hence there are two dynamical equations, derived from the energy and mass balance. We will first give the two equations, and then we will explain and justify each term by giving heuristic and ecologically intuitive arguments. The dynamics is basically given by four fluxes, denoted with  $F$ :

$$\frac{dU}{dt} = C_V \frac{dT_E}{dt} = F_H - F_E$$

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<sup>3</sup>For more realistic systems, like e.g. the earth, there are different biotic species  $B_i$  and different temperatures. If spatial diffusion of biota and heat is included, it allows to study spatial patterns, but we will leave that for future research.

$$= \alpha_H(T_H^0)^4 - \epsilon_L T_E^4 \quad (8.1)$$

$$\begin{aligned} \frac{dB}{dt} &= F_{gBH} - F_{dB} \\ &= g_B B(1 - B)(T_H^0)^4 - d_B B \end{aligned} \quad (8.2)$$

The first equation is the energy balance for the ecosystem, with  $U$  the internal heat energy and  $C_V$  the heat capacity at constant volume (which might be dependent on the variable  $B$ ). The heat balance is simply given by the absorption minus the emission flux.

The absorption flux  $F_\alpha$  of high temperature (high frequency) radiation from the source to the ecosystem is proportional with the temperature factor  $(T_H^0)^4$ , which is characteristic for grey or black body radiation. The prefactor

$$\alpha_H \equiv (\alpha_{HA}(1 - B) + \alpha_{HB}B) \quad (8.3)$$

contains the constant parameter  $\alpha_{HA}$ , which depends on universal physical constants (Stefan-Boltzmann constant, the velocity of light), geometric factors (the areas of the source and the ecosystem, the distance between source and ecosystem and the inclination of the system surface) and the albedo (reflectivity)  $a_A \leq 1$  of the abiotic elements. An exact expression of the parameter  $\alpha_{HA}$  is not relevant for our discussion (interested reader is referred to [156] for a simple example). The factor  $(1 - B)$  is added because there is competition for light capture (space) between biotic and abiotic elements: Biota can cover (shade) or replace the abiotic elements<sup>4</sup>. These biota can have a different parameter,  $\alpha_{HB}$ , because the biota can have a different albedo ( $a_B$ ) than the abiotic elements. Both abiotic and biotic albedos form the ecosystem albedo ( $a_E = (1 - B)a_A + Ba_B$ ).

For modeling simplicity, we impose a few important assumptions: The source is a black body radiator, and the  $\alpha_{HA}$  and  $\alpha_{HB}$  factors are independent of the biotic fraction  $B$ , the temperatures ( $T_H^0$ ,  $T_E$  or  $T_L^0$ ) and the frequency. These approximations might be too strong for real ecosystems<sup>5</sup>, but as the focus lies primarily on the theoretical concepts, we shall use these simplifications as a starting point. Refinements are reserved for later studies.

The outflux  $F_E$  of low frequency radiation from the ecosystem to the background contains the emissivity factor  $\epsilon_L$ , which is frequency independent but contains physical constants and geometric factors, as well as the emissivity  $e_E \leq 1$ . However, for reliable EP expressions, we will assume that the ecosystem is a black body, and the emitted radiation has well defined temperature  $T_E$ . As  $e_E = 1$  is constant, there are no biotic effects on the emissivity. This assumption means that the abiotic and biotic elements behave together in such a way that the total emitted spectrum is always a black body radiation (for all values of  $B \in [0, 1]$ ).

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<sup>4</sup>We assume that a reflected or transmitted photon travels immediately to the background. Otherwise, it would be possible that (a)biotic elements reflect or transmit high frequency radiation that is consequently absorbed by other (a)biotic elements. Modeling this property can be done by using e.g. the factor  $(1 - f(B))$ , with a more complex function  $f(B)$ . When  $f(1) \leq 1$ , complete cover ( $B = 1$ ) in a terrestrial system might still allow some abiotic absorption, due to the transmittivity of the biota. These more complex functional dependences should be studied in future research.

<sup>5</sup>E.g. the albedo of a leaf is highly frequency dependent in the visible light range, explaining why it is green rather than grey. Also the independence of  $T_H^0$  might be invalid.

As a final remark regarding the energy balance equation, note that the source drives the system far out of equilibrium, so there should be a constraint

$$\alpha_H \ll \epsilon_L \quad (8.4)$$

because  $T_H^0 \gg T_E^*$  in the steady state for  $T_E$  (steady states are denoted with a \*).

The growth rate is denoted with  $F_{gBH}$  for the fraction  $B$  on the high frequency irradiation.  $g_B = g'_B \alpha_B$  is the constant effective growth rate parameter. When the albedo is 1 (i.e.  $\alpha_B = 0$ ), the biota do not absorb light, and growth should be impossible.  $g'_B$  is the intrinsic growth rate parameter. The growth (by photosynthesis) is also dependent on the wavelength of the irradiation, and hence on the temperature of the source. For simplicity<sup>6</sup> we use the factor  $(T_H^0)^4$ , because in this way the growth is proportional with the net irradiation of a black body source. Due to autocatalytic feedback, the growth should be proportional with  $B$ , but intraspecific competition for space or nutrients means that  $B = 1$  is the maximum. Therefore, we have included a logistic growth factor  $(1 - B)$ .

Finally, the biotic decay rate is  $F_{dB}$ , with  $d_B$  the constant decay rate parameter.

This concludes the description of the phototrophic model, which is a version of a Daisyworld model [203], with one energy balance for both biota and non-biota (they have the same temperature  $T_E$ ), a biotic dependence on the absorptivity, one daisy species and no temperature feedbacks ( $T_E$  dependence) for the growth and decay. As the ecosystem description is homogenized, it is a 'zero-dimensional' Gaia model: information on spatial structure and dynamics was not incorporated.

### 8.4.3 The steady states and the bifurcation

We will now look at the steady states (denoted with a superscript \*) of the equations (8.1-8.2). We first define the thermodynamic gradient

$$\Delta \equiv (T_H^0)^4. \quad (8.5)$$

This is basically a parameter that measures how far the environment (containing source and background) is out of equilibrium. (Note that  $T_L^0$  is absent in  $\Delta$ , because it is negligible.) It is this gradient which is applied to the system and which drives the biological growth. There is a critical level for the gradient

$$\Delta_c = d_B/g_B. \quad (8.6)$$

When the gradient has a value below this critical level, there is only one physical steady state, which is abiotic

$$(T_{EA}^*)^4 = \frac{\alpha_{HA}}{\epsilon_L} \Delta, \quad (8.7)$$

$$B_A^* = 0. \quad (8.8)$$

---

<sup>6</sup>For photosynthetic organisms, this fourth power functionality on the temperatures might be (highly) unrealistic. In order to obtain simple, analytic solutions, we will stick to our expression (8.2), but we keep in mind that this postulated expression is possibly the weakest point in our model. Therefore, refinements in later studies are welcome.

But if  $\Delta \geq \Delta_c$ , there are two steady states: the above abiotic (unstable) one and a biotic (stable) state:

$$(T_{EB}^*)^4 = \frac{\alpha_{HA}}{\epsilon_L} \Delta \left[ \left( 1 - \frac{d_B}{g_B \Delta} \right) \frac{\alpha_{HB}}{\alpha_{HA}} + \frac{d_B}{g_B \Delta} \right], \quad (8.9)$$

$$B_B^* = 1 - \frac{d_B}{g_B \Delta}. \quad (8.10)$$

By looking at (8.6), we can observe our first interesting result: When  $d_B \rightarrow 0$ , we have  $\Delta_c \rightarrow 0$ , meaning that in this limit life can survive arbitrarily close to equilibrium. Hence, the statement that life is a dissipative structure with non-trivial bifurcation point, is highly dependent on the functionality in  $B$  of the decay term. When this term is linear in  $B$ , phototrophic life has the correct bifurcation property. But would it be absent or of higher order (e.g.  $d_B B^2$ ) phototrophic life would not be a dissipative structure. It is interesting to note that the second law of thermodynamics is not responsible for the (non-)triviality of the bifurcation point. The second law only says that the EP of an irreversible process should be positive, but that does not give restrictions on the functionality or even the presence or absence of a process.

#### 8.4.4 The entropy production

We are now going to study the EP in the steady state(s). As the ecosystem is materially closed, and as  $B^*$  is constant in the steady state, there is no EP contribution from changing  $B$ . The entropy balance gives an expression for the EP, which was used by e.g. Kleidon [85]:

$$\sigma_{HE}^* = \alpha_H^* \Delta \left( \frac{1}{T_E^*} - \frac{1}{T_H^0} \right). \quad (8.11)$$

This EP is the product of the irradiation (absorption) heat energy flux  $F_\alpha$  and the thermodynamic force  $X = \left( \frac{1}{T_E} - \frac{1}{T_H^0} \right)$ . This basically means that heat energy at temperature  $T_H^0$  is turned into heat at temperature  $T_E$ .

For both abiotic and biotic states we can write for the fluxes and the forces

$$F_{\alpha,A}^* = \alpha_{HA} \Delta, \quad (8.12)$$

$$F_{\alpha,B}^* = \alpha_{HA} \Delta \left[ 1 - \left( 1 - \frac{d_B}{g_B \Delta} \right) \left( 1 - \frac{\alpha_{HB}}{\alpha_{HA}} \right) \right]. \quad (8.13)$$

$$X_A^* = \frac{1}{\Delta^{1/4}} \left[ \sqrt[4]{\frac{\epsilon_L}{\alpha_{HA}}} - 1 \right], \quad (8.14)$$

$$X_B^* = \frac{1}{\Delta^{1/4}} \left[ \sqrt[4]{\frac{\epsilon_L}{\alpha_{HA}} \left( \frac{g_B \Delta}{(g_B \Delta - d_B)(\alpha_{HB}/\alpha_{HA}) + d_B} \right)} - 1 \right]. \quad (8.15)$$

With the above expressions for the EP as flux times force, one can easily see when life is ultra or infra dissipative. Looking at  $F_\alpha^*$ , we notice that when  $\frac{\alpha_{HB}}{\alpha_{HA}} \leq 1$ , the biotic state (for  $\Delta \geq \Delta_c$ ) has a lower energy capture than the abiotic state. For the moment, there is no physical law (like e.g. the second law) known that forbids this possibility. The claim by Schneider et al. [179] and Lotka [99] that biotic states maximize energy capture and energy throughflow

would be a new ecological law. But a priori one can think of a dead ecosystem which is black in the high frequency visible spectrum (ecosystem albedo  $a_E = 0$ ), and a living state consisting of biota which are 'grey' or colored ( $0 < a_E < 1$ ), contradicting this new ecological law.

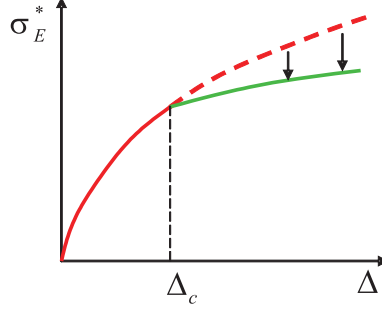


Figure 8.2: Infra dissipation. The qualitative behavior for the ecosystem steady state EP as a function of the gradient in the phototrophic system. The dashed curve represent the unstable states and the solid curves the stable states. Red is abiotic, green is biotic.

As for the EP behavior, we obtain a curious result. Define  $f \equiv \alpha_{HB}/\alpha_{HA}$ , i.e. the ratio of the biotic and abiotic absorptivities, and write the EP in function of  $f$ . If  $f = 1$ , we obtain nothing but the abiotic EP. We can also show that

$$f \in \left[ 0, \frac{\epsilon_L - \alpha_{HA}d_B/g_B\Delta}{\alpha_{HA}(1 - d_B/g_B\Delta)} \right]. \quad (8.16)$$

The upper limit should be larger than 1, and hence  $\epsilon_L \geq \alpha_{HA}$ , which we already knew (8.4). Let us now search for the value  $f_{MaxEP}$  whereby the EP  $\sigma_{HE}^*(f)$  becomes maximal. Taking the extremum of the EP with respect to  $f$  (at constant  $\alpha_{HA}$ ) we obtain after some calculations the remarkable expression

$$f_{MaxEP} = \frac{81\epsilon_L - 256\alpha_{HA}d_B/g_B\Delta}{256\alpha_{HA}(1 - d_B/g_B\Delta)}. \quad (8.17)$$

Refereing to the maximum EP discussions in e.g. [85, 86], we can postulate a 'biotic absorptivity' MaxEP hypothesis, but that will not be our focus here. We are primarily interested in the possibility for infra-dissipative behavior. A curious property is that if the abiotic emission and absorption factors are related as  $\epsilon_L = (256/81)\alpha_{HA}$ , then  $f_{MaxEP} = 1$ . Consequently, in this particular situation, every value for  $f$ , and hence every value for the biotic absorptivity, leads to a biotic EP which is *lower* than the abiotic counterpart, i.e. life is an infra dissipative structure (see fig. 8.2).

To compare this with the sun-earth system, we have  $\alpha_{HA}/\epsilon_L = (T_E/T_H^0)^4 \sim 4.10^{-6} \ll 81/256$ , or  $f_{MaxEP} \gg 1$ . Hence for the sun-earth system, life would be infra-dissipative once  $f < 1$ , or  $\alpha_{HB} < \alpha_{HA}$ . We can conclude that for this model, it seems easy to find parameter values whereby life is infra-dissipative. The abiotic and biotic elements both turn a low number of captured high frequency photons in a large number of low frequency photons. This turnover produces entropy, but a priori it is possible that this turnover is lower for the biota, resulting in a lower EP. In the concluding section we will comment further on the implications of this result.

## 8.5 The chemotrophic ecosystem

Let us now study a chemotrophic ecosystem, which is a resource consumer model as discussed in chapter 4, but with one crucial extension: The exchange rate  $\alpha_R$  is no longer a constant, but might depend on the consumer concentration. This exchange rate is the analogue of the absorptivity factor in the phototrophic model. To obtain interesting biotic feedbacks, similar to the phototrophic 'Gaian' feedback in the previous model, we will write this rate as

$$\alpha_R = \alpha_{AR} - l_C C_C \quad (8.18)$$

Hence, this rate includes an abiotic term  $\alpha_{AR} \geq 0$  and a biotic one  $-l_C C_C$ . The latter term is a biotic exchange limitation ( $l_C \geq 0$ ) or enhancement ( $l_C \leq 0$ ). Limitation is possible when e.g. the biota are silting up the resource input valve in a chemostat reactor tank. An example of enhancement occurs in e.g. filter feeding of aquatic bioturbative sediment ecosystems [118].

### 8.5.1 The steady states and the bifurcation

The quantity that measures the distance from thermodynamic equilibrium is the gradient

$$\Delta \equiv C_R^0 - C_W^0 / K_{eq}. \quad (8.19)$$

Solving the dynamics for the steady states, we see that there is a critical gradient level

$$\Delta_c = \left( \frac{\alpha_{AR} + \kappa_{AC}}{\alpha_{AR}} \right) \frac{d_C}{q_{CR} g_{CR}} \quad (8.20)$$

The physical, abiotic steady state for a gradient value  $\Delta \leq \Delta_c$  is

$$C_{RA}^* = \frac{\alpha_{AR}}{\alpha_{AR} + \kappa_{AC}} \Delta + \frac{C_W^0}{K_{eq}}, \quad (8.21)$$

$$C_{CA}^* = 0. \quad (8.22)$$

The biotic state is unphysical because it has negative concentrations.

When  $\Delta \geq \Delta_c$ , there are two realistic steady states, the abiotic (unstable) one from above and the biotic (stable):

$$C_{RB}^* = \frac{d_C}{q_{CR} g_{CR}} + \frac{C_W^0}{K_{eq}}, \quad (8.23)$$

$$C_{CB}^* = \frac{\alpha_{AR} q_{CR} g_{CR} \Delta - (\alpha_{AR} + \kappa_{AC}) d_C}{l_C q_{CR} g_{CR} \Delta - (l_C - g_{CR}) d_C}. \quad (8.24)$$

In order to keep  $C_C^*$  finite and positive, we need as extra constraint

$$l_C > -\frac{g_{CR} d_C}{q_{CR} g_{CR} \Delta - d_C}. \quad (8.25)$$

(This constraint would be absent when we include an intraspecific competition term  $-m_C C_C^2$  in the dynamics for the consumer.)

Again, as in the phototrophic system, we notice the interesting property that there is a non-trivial bifurcation point  $\Delta_c \neq 0$  when  $d_C \neq 0$ , and that this bifurcation point is highly dependent on the functionality, as e.g. a term like  $d_C C_C^2$  would result in a trivial bifurcation point  $\Delta_c = 0$ .

### 8.5.2 The entropy production

We are now ready to study the behavior of the EP in our chemotrophic ecosystem, in order to solve the question: "Is chemotrophic life ultra or infra dissipative?" The steady state total EP  $\sigma_{tot}^* = F^* X^0$  with the flux

$$F^* = F_R^* = (\alpha_{AR} - l_C C_C^*)(C_R^0 - C_R^*), \quad (8.26)$$

and the thermodynamic force

$$X^0 = R \ln \frac{C_R^0 K_{eq}}{C_W^0} = R \ln \left( \frac{K_{eq} \Delta}{C_W^0} + 1 \right). \quad (8.27)$$

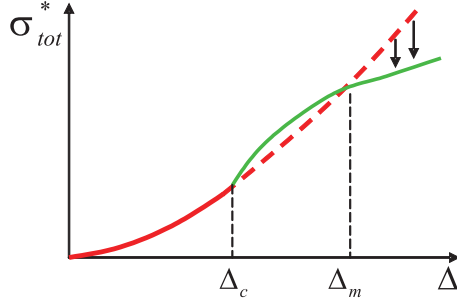


Figure 8.3: Infra dissipation. The qualitative behavior of the total steady state EP as a function of the gradient in the chemotrophic system, for  $0 \leq l_C \leq \alpha_{AR}^2 g_{CR} / \kappa_{AC}^2$ . The dashed curve represent the unstable states and the solid curves the stable states. Red is abiotic, green is biotic.

For fixed gradients  $\Delta$ , the total steady state EP is proportional with the total flux  $F_R^*$ . The abiotic and biotic fluxes are

$$F_{RA}^* = \frac{\alpha_{AR} \kappa_{AC}}{\alpha_{AR} + \kappa_{AC}} \Delta, \quad (8.28)$$

$$F_{RB}^* = \frac{(\alpha_{AR} g_{CR} + l_C \kappa_{AC}) d_C}{l_C q_{CR} g_{CR} \Delta - (l_C - g_{CR}) d_C} \left( \Delta - \frac{d_C}{q_{CR} g_{CR}} \right). \quad (8.29)$$

When  $l_C > 0$ , we see that for  $\Delta$  large enough, the stable biotic flux becomes *lower* than the unstable abiotic flux, because the biotic flux reaches a constant, and the abiotic flux increases linearly in  $\Delta$ . The same happens for the EP. In fact, one can easily show that if  $l_C \geq l_C^o$ , with

$$l_C^o = \alpha_{AR}^2 g_{CR} / \kappa_{AC}^2, \quad (8.30)$$

then the EP in the biotic state (for  $\Delta \in [\Delta_c, \infty[$ ) is always lower than the EP in the corresponding abiotic state, meaning that under this condition chemotrophic life is always infra dissipative. When  $l_C \leq l_C^o$ , there is a regime  $\Delta \in [\Delta_c, \Delta_m]$  where the biotic EP is higher than the abiotic, and a regime  $\Delta \in [\Delta_m, \infty[$  where the biotic EP is lower (see fig. 8.3). Note that when  $l_C = 0$ , chemotrophic life is always ultra dissipative.

## 8.6 Conclusions and further discussion

We have studied both phototrophic and chemotrophic ecosystems, solved the dynamical equations to derive the steady states, wrote down expressions for the EP and discussed criteria to see whether the biotic state is ultra or infra dissipative. At the theoretical level, the second law of thermodynamics nor any other physical law does a priori exclude some values for the parameters that lead to infra dissipative states. The second law only restrict the parameters to have the correct sign (e.g.  $\alpha_{AR} \geq 0$ ) for the EP to be positive.

Whether the infra dissipative behavior is possible in real life is for the moment a question for the experimentalist. Up till now, no clear example of an infra dissipative system is found. E.g. sediment ecosystems have typically resource exchange enhancement ( $l_C \leq 0$ ) due to bioturbation [118] whereas it is the exchange limitation that results in infra dissipative behavior.

Also phototrophic biota might indicate ultra dissipative behavior [85]. Plants have often a lower albedo than sand and dry soil [25], which results in  $\alpha_{HB} > \alpha_{HA}$  and a higher energy capture  $F_{H,B}^*$  (8.13) and EP. But this is not always true: e.g. in the tropical forests, the forest albedo is higher than the underlying dark wet soil.

As some open questions for future research, one might ask whether evolution has an impact on our results. Suppose one of the biota mutates into a new organism. The biotic steady state might shift towards a new value (as happens in the competitive exclusion principle [7]), and consequently the EP might also change. Is there a preference for ever higher EP values under the process of evolution? Speculating further, does this lead to a biotic absorptivity MaxEP, with life as a 'maximal dissipator'?

Another open problem is the study of grey body ecosystems, or even more general ecosystems with more complex emissivities. E.g. for the earth system as a whole, the effect of life on greenhouse gases is an important factor for the total earth emissivity. And although the tropical forest might have a higher albedo than the soil, due to e.g. an increased evapotranspiration, there might be an extra contribution to the emissivity, turning the forest ecosystem in an ultra dissipator. One can intuitively argue that the biotic emissivity should be much larger than the abiotic emissivity. Looking at biotic processes (photosynthetic reactions,...), they often involve an energy 'cascade' of excited molecules moving down to lower energy levels by emitting radiation. Roughly speaking, the more steps on the energy staircase, the more photons are emitted and the higher becomes the emissivity. As biotic chemical reactions are typically much more complex (with longer energy cascades) than abiotic absorption and emission, one might generally expect that the biotic emissivity is typically higher than the abiotic one.

When true, the statement that life on earth is always ultra [199] or even maximal [78, 85, 191] dissipative, would be a new (ecological) law. A simple analogy can clarify the meaning of this result. Take e.g. a self-replicating molecule. There is a priori no restriction on the number of atoms in the molecule, apart from the physical constraint that the number of atoms should be positive (to see the analogy, call this the 'second law of molecules'). But for the molecule to be able to replicate itself, it should be sufficiently complex, which requires a sufficient amount of molecules. In other words, there is a non-trivial lower bound on the number of atoms required for self-replication. Also the EP of

life might have a non-trivial lower bound (the trivial lower bound is imposed by the second law of thermodynamics). When this lower bound is above the abiotic EP, life is ultra dissipative, and this property might have potentially far reaching implications.

## Chapter 9

# A useful correspondence between fluid convection and ecosystem operation

### Abstract<sup>1</sup>

Both ecological systems and convective fluid systems are examples of open systems which operate far-from-equilibrium. Here we will demonstrate that there is a correspondence between a resource-consumer chemostat ecosystem and the Rayleigh-Bénard (RB) convective fluid system. The Lorenz dynamics of the RB system can be translated into an ecosystem dynamics. Not only is there a correspondence between the dynamical equations, also the physical interpretations show interesting analogies. By using this fluid-ecosystem analogy, we are able to derive the correct value of the size of convection rolls by competitive fitness arguments borrowed from ecology.

### 9.1 Introduction

In a Rayleigh-Bénard experiment, a horizontal viscous fluid layer is heated from below. When the temperature difference between upper and lower sides is small, heat transfer solely occurs through thermal conduction. Yet once beyond a critical temperature difference, a regular pattern of convection cells or rolls emerges [14]. This sudden shift from conduction to convection is referred to as the Rayleigh-Bénard (RB) instability, and is often quoted as an archetypal example of self-organization in non-equilibrium systems [135, 159].

Intuitively, it makes sense to try to apply the concept of self-organization in physical non-equilibrium systems to ecological systems, as there are similarities between ecological and physical systems. Like the Rayleigh-Bénard set-up, ecosystems are open systems that receive a throughput of energy and/or mass via coupling to an environment [125, 182]. The environment typically consists of two large reservoirs, and the difference of a thermodynamic quantity (e.g. the temperature) of these reservoirs drives the system from equilibrium. Consider the example of a laboratory chemostat ecosystem [185]. This is a prime

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<sup>1</sup>This chapter is based on an article in progress [222].

example of a chemotrophic ecosystem whereby a resource of energetic high quality chemical substrate is pumped from an external reservoir into the system. In the ecosystem this resource is degraded into low quality waste products which are emitted to the waste reservoir. When there is low supply of resource, no biota can survive, and the resource is degraded by abiotic processes only. But when the supply is above a critical threshold, biota can survive by consuming the resource. There is a sudden shift from a non-living to a living state<sup>2</sup>. In other words, the energetic quality difference between incoming and outgoing chemical substrates is exploited by various abiotic and biotic processes. The latter biotic processes contain the biomass synthesis and turnover of consumer micro-organisms feeding on the resource.

So it is tempting to look for a deeper connection. Can one compare biological resource processing with convection? Both mechanisms involve self-organizing structures, biological cells or convection cells, that can only survive after a critical threshold of an environmental driving force. Both energetic pathways, biotic resource conversion and thermal convection, degrade energy from high quality to low quality form. And these energetic pathways are additional to the abiotic conversion or thermal conduction processes of the background.

Here, our ambition is to examine the link between ecological processes and convective fluid motions in a quantitative way. The first part contains a highly intriguing result: The mathematical expressions of the resource-consumer chemostat ecosystem dynamics are exactly the same as the dynamics that describe the basics of the Rayleigh-Bénard system. Furthermore, not only are the mathematical equations identical, also the physical/ecological interpretations give appealing results. Particularly, by looking at the energetic pathways of the ecosystem, the ecological quantities can be mapped one to one to the quantities used in the fluid system.

The second part tries to extend the correspondence between fluid convection and ecosystem functioning to include competition. One can look at ecological competition and translate the notion of competitive fitness to the fluid system. The convection cells are in 'Darwinian competition' with each other and the fittest ones will survive. One can generalize the Lorenz model to include this fluid competition. As the size of a convection cell will depend on the fluid fitness measure, we will demonstrate that the mathematical identity of the ecological and the fluid dynamics predicts the experimentally correct size of the cells at the onset of convection.

## 9.2 The Rayleigh-Bénard convection system

Let us start by deriving the dynamics that describes the Rayleigh-Bénard (RB) convective fluid system, named after Bénard [14] and Rayleigh [162] who were the first to study this system experimentally and theoretically. A full mathematical treatment of thermal convection requires the combined solution of the heat transport, Navier-Stokes and incompressibility equations, resulting in a set of five coupled non-linear partial differential equations [33].

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<sup>2</sup>Strictly speaking, it is rather a distinction between guaranteed extinction and survival. We study what will happen with an organism which is released in the ecosystem. Our results should not be interpreted as the solution for the origin of life problem.

Rather than solving this full set, we employ the approximation adopted by Lorenz [97], which became famous as it gave an new impulse to the development of chaos theory. The model describes the lowest modes of an expansion of the temperature and velocity fields for a RB system with free-free boundary conditions (see e.g. [63]). In appendix 9.9, the derivation of the Lorenz system is given in a way that will suit our further discussion. A non-linear set of three ordinary differential equations is obtained, with three variables (see fig. 9.1):  $X$  measures the rotation rate of the rolls and represents the maximal velocity at the bottom of the rolls.  $Y$  and  $Z$  are temperature deviations, where the linear profile of the conduction state is taken as a reference.

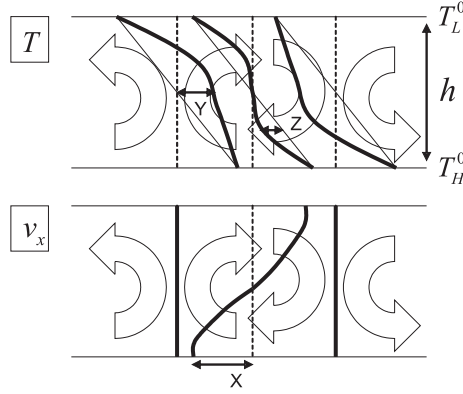


Figure 9.1: The profiles and the variables  $X$ ,  $Y$  and  $Z$ . The temperature ( $T$ ) and horizontal velocity ( $v_x$ ) profiles at three vertical sections (dashed lines) are shown. These vertical sections are parallel with the axes of the convection rolls, where the fluid is moving up, moving horizontal or moving down. The thin linear profiles correspond with the conduction state, the thick profiles with the convection state. As indicated,  $Y$  and  $Z$  are temperature deviations and  $X$  is the velocity at the bottom of a roll.

With these three variables, the XYZ Lorenz system is rich enough to describe the Rayleigh-Bénard instability, the sudden shift from conduction to convection. But there is an even simpler model, the XZ system with only two variables, that is rich enough as well. It is this XZ model that allows us to make the correspondence. Roughly speaking, we will perform a kind of averaging over the horizontal directions, such that only the average vertical profile remains. As  $Y$  is the temperature deviation in horizontal direction (the temperature difference between ascending and descending fluid), it is this variable that will disappear after the 'averaging'. More specifically, this is done by making the pseudo steady state assumption  $dY/dt = 0$  for the variable  $Y$ . The latter becomes a constant and the dynamics turns into:

$$\frac{dX}{dt} = \left( \frac{a^2 h^2 g \alpha}{(a^2 + 1)^2 \pi^2 \chi} - \frac{(a^2 + 1) \pi^2 \nu}{h^2} \right) X - \frac{2a^2 h g \alpha}{(a^2 + 1)^2 \pi^2 \chi} XZ, \quad (9.1)$$

$$\frac{dZ}{dt} = \frac{a^2 \pi \beta}{2(a^2 + 1) h \chi} X^2 - \frac{a^2 \pi^2}{(a^2 + 1) h^2 \chi} X^2 Z - \frac{4\pi^2 \chi}{h^2} Z, \quad (9.2)$$

with  $h$  the height of the fluid layer,  $a$  a geometric factor (such that  $h/a$  is the width of the straight convection rolls),  $\alpha$  the thermal expansion coefficient,  $g$

the gravitational acceleration,  $\chi$  the heat conduction coefficient,  $\nu$  the kinematic viscosity and

$$\beta = \frac{T_H^0 - T_L^0}{h} \quad (9.3)$$

the temperature gradient. This important quantity is the thermodynamic gradient that drives the system out of equilibrium.  $T_H^0$  is the high temperature of the heat reservoir below the fluid layer and  $T_L^0$  is the low temperature of the heat reservoir above the layer.

For further reference, we will also need measures for the temperatures at the middle and the lower half of the fluid layer. Define

$$T_M^0 \equiv \frac{T_H^0 + T_L^0}{2} \quad (9.4)$$

as the horizontally average temperature at height  $h/2$ , and

$$T_H \equiv \frac{T_H^0 + T_M^0 - \pi Z}{2}. \quad (9.5)$$

Fig. 9.2 shows the interpretation of  $T_H$  as a temperature measure for a linearized temperature profile in the lower half of the fluid layer. (Due to symmetry in the approximation leading to the Lorenz system, we will not have to include the upper half of the fluid layer.)

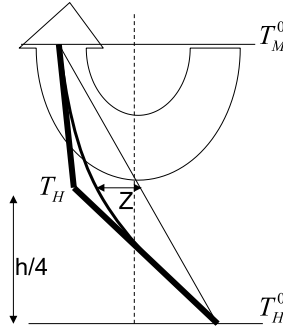


Figure 9.2: The definition of  $T_H$ . The lower half of the fluid layer is shown, with the vertical (horizontally averaged) temperature profiles in the conduction state (thin line), the convection state (thicker line) and the 'linearized' convection profile (thickest line). The variables  $Z$  and  $T_H$  are measured at height  $h/4$ .

### 9.3 The resource-consumer ecosystem

Next, we discuss the ecosystem model, which is in essence a simple chemotrophic resource-consumer food web model, one of the mainstay models of ecology [210]. Consumer organisms are feeding on some food resource (R), which is partly converted to consumer biomass (C) and partly to waste product (W). For reference, one can think of a chemostat set-up where a chemical reactor tank contains a monoculture of micro-organisms that are feeding on a chemical substrate like methane or glucose, while respiring  $CO_2$ .

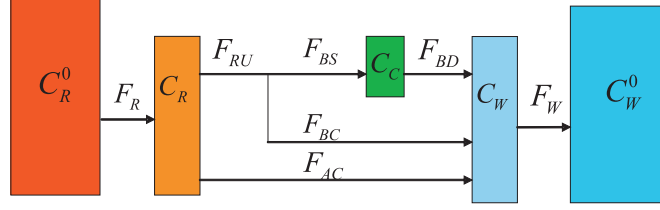


Figure 9.3: The ecosystem flow chart. The resource-consumer-waste ecosystem coupled with the two environments. The different fluxes are discussed in appendix 9.8. The color denotes the 'energetic quality' of the substances, from high (red) to low (light yellow).

Figure 9.3 gives a schematic overview of the ecosystem coupled with the two environmental reservoirs (denoted with the superscripts 0). The two environmental compartments have a constant resource concentration  $C_R^0$  and a constant waste concentration  $C_W^0$ . The three ecosystem compartments have variable concentrations  $C_R$ ,  $C_C$  and  $C_W$  for the resource, the consumer biomass and the waste respectively. In appendix 9.8, the complete dynamics of the resource-consumer-waste (RCW) ecosystem is given, explaining the fluxes  $F$  between the compartments.

However, as we will see, the correspondence only works in a limiting case, whereby roughly speaking we will average over the waste concentrations of the system and the environment. Specifically, this can be done by taking a very small relaxation time for the exchange of the waste between the ecosystem and the reservoir. This means that by studying the ecosystem at longer time scales than this relaxation time, the dynamics for  $W$  is forced to be in a pseudo steady state condition. Hence,  $C_W$  is no longer a variable and we end up with the resource-consumer (RC) model, with two dynamical equations for two remaining variables:

$$\frac{d}{dt}C_R = \alpha_R(C_R^0 - C_R) - (\kappa_{AC} + g_{CR}C_C)(C_R - C_W^0/K_{eq}), \quad (9.6)$$

$$\frac{d}{dt}C_C = q_{CR}g_{CR}(C_R - C_W^0/K_{eq})C_C - d_C C_C, \quad (9.7)$$

with,  $\alpha_R$  the resource exchange rate parameter,  $\kappa_{AC}$  the abiotic conversion (from R to W) rate parameter,  $g_{CR}$  the consumer growth rate parameter,  $q_{CR}$  the yield factor for the consumer growth,  $d_C$  the consumer decay (basal maintenance) rate parameter, and  $K_{eq}$  the equilibrium constant for the chemical reaction (oxidation) from R to W which always slowly proceeds at the background.

This is the well-known chemostat dynamics [185], which is extended in two ways: First, abiotic conversion is included in terms of chemical oxidation with parameters  $\kappa_{AC}$  and  $C_W^0/K_{eq}$ . Second, instead of the classical dependence of the growth on the resource  $C_R$ , the growth is now made dependent on  $C_R - C_W^0/K_{eq}$ . This is done for thermodynamic consistency: at chemical equilibrium, biomass synthesis should also cease.

Let us summarize. Table 9.1 shows the observation that there are two systems with analogous mechanisms for the degradation of a gradient, i.e. the transformation of high quality energy to low quality energy. The unstructured processes are the ground level mechanisms: abiotic conversion from resource to

	ecosystem	fluid system
unstructured & structured gradient degradation	abiotic & biotic metabolism	conductive & convective heat transport
structures	biological organisms	convection patterns
model	RC	XZ

Table 9.1: Two corresponding models with analogous mechanisms for gradient degradation

waste or thermal conduction from high temperature to low temperature. But above a certain critical threshold, a self-organization mechanism adds second level processes: biotic conversion or thermal convection.

To study these systems, we introduced two models, each with three variables: the XYZ Lorenz model (one velocity  $X$  and two temperatures  $Y$  and  $Z$ ) and the RCW ecosystem model (one biotic consumer  $C$  and two abiotic compounds  $R$  and  $W$ ). These systems have different behavior, as the XYZ model has chaotic solutions whereas they are absent in the RCW model. However, there is a hidden correspondence which we will clarify in the next section. We have to make a pseudo steady state condition (an averaging) of the 'abiotic' variables  $Y$  and  $W$ , leading to the XZ model (9.1-9.2) and the RC model (9.6-9.7). These models have only two variables and hence they are the most simple models to study a non-trivial behavior, the transition from an 'abiotic' to a 'biotic' state. The XZ system does not have chaotic solutions anymore, so it is possible that it is mathematically equivalent with the RC model. The trick is to rewrite the variables and the parameters to demonstrate this equivalence. To give a first hint, the basic observation is that the variables should be related as

$$C_R - \frac{C_W^0}{K_{eq}} \leftrightarrow \frac{h\beta}{4} - \frac{\pi}{2}Z, \quad (9.8)$$

$$C_C \leftrightarrow \frac{X^2}{g\alpha h^3}. \quad (9.9)$$

Note that the quantities on the right hand side have dimensions of temperature. In the next section, we will also relate the parameters and discuss the physical interpretations of this correspondence

## 9.4 The correspondence

So it is time to write the dictionary of the correspondence. Our final result is shown in table 11.3 at the end. In order to reach our goal, we need to be able to consistently translate quantities from one system to the other. The redefinitions explained below enable us to write the simplified Lorenz dynamics as the ecosystem dynamics.

First we will state the relation between the basic quantities, the concentrations and the temperatures, which is simply:

$$C_R^0 \leftrightarrow T_H^0, \quad (9.10)$$

$$C_R \leftrightarrow T_H, \quad (9.11)$$

$$\frac{C_W^0}{K_{eq}} \leftrightarrow T_M^0. \quad (9.12)$$

These were derived by using (9.8) and the interpretation of  $T_H$  (9.5). It explains why we can roughly interpret the resource as the heat energy.

The consumer concentration is given by (9.9). As  $X$  is a velocity measure,  $X^2$  is a measure for the kinetic energy of the convection rolls. This kinetic energy is consuming the heat energy resource.

The yield and consumer growth parameters are written as

$$q_{CR} \leftrightarrow \frac{8}{\pi^4(a^2 + 1)}, \quad (9.13)$$

$$g_{CR} \leftrightarrow \frac{g\alpha ha^2\pi^2}{(a^2 + 1)\chi}. \quad (9.14)$$

As the gravitational field is causing the buoyancy force, this explains why  $g$  appears in  $g_{CR}$ . Furthermore, these parameters depend on geometric factors, especially  $a$  that determines the relative width of a convection roll. The importance of this dependence will be shown later.

The abiotic exchange and abiotic conversion parameters are

$$\alpha_R = \kappa_{AC} \leftrightarrow \frac{2\pi^2\chi}{h^2}. \quad (9.15)$$

As these parameters are conduction coefficients, it is logical that they depend on the heat conduction coefficient  $\chi$ . In order that the analogy works, our ecosystems should have equal exchange and abiotic conversion parameters<sup>3</sup>.

The final parameter is the biomass decay rate

$$d_C \leftrightarrow \frac{2(a^2 + 1)\pi^2\nu}{h^2}. \quad (9.16)$$

This explains why this decay is a kind of friction term. As mortality and viscous friction destroy the biological or convective cells, a continuous feeding on the resource is required in order that these structures can survive.

Having discussed the relations between variables and parameters of both systems, one can take a look at other ideas and concepts of one system and translate it to the other. A quantity that will become useful later is the thermodynamic gradient that measures how far the system is out of equilibrium. It is given by the difference in energetic 'quality' of the two reservoirs.

$$\Delta^0 \equiv C_R^0 - \frac{C_W^0}{K_{eq}} \leftrightarrow \frac{h\beta}{2} = (T_H^0 - T_M^0). \quad (9.17)$$

The latter relation can be turned into a dimensionless measure, which is the well known Rayleigh number  $Ra$  in fluid systems. Another important dimensionless

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<sup>3</sup>The reason is that we identified (9.11), and the distance between the lower side and height  $h/4$  equals the distance from this height to the middle of the fluid layer. As we will see in chapter 10, there is a possibility to have a more general correspondence, with  $\alpha_R \neq \kappa_{AC}$ , but then we will loose the relation (9.11).

fluid quantity is the Prandtl number  $Pr$ . We can now see that they can be casted into their ecological analogs:

$$Ra \equiv \frac{g\alpha h^3(T_H^0 - T_L^0)}{\nu\chi} \leftrightarrow G \frac{q_{CR}g_{CR}\Delta^0}{d_C}, \quad (9.18)$$

$$Pr \equiv \frac{\nu}{\chi} \leftrightarrow H \frac{d_C}{\alpha_R + \kappa_{AC}}. \quad (9.19)$$

The geometric factors

$$G = \frac{(a^2 + 1)^3 \pi^4}{2a^2}, \quad (9.20)$$

$$H = \frac{a^2 + 1}{2} \quad (9.21)$$

will become important later on.

This is the first part of our dictionary. In the next section we will delve deeper into the physical analogies between both systems. In particular, we will look at the energy dissipation along the different energetic pathways.

## 9.5 Energy flows along energetic pathways

Our next challenge is to see whether the correspondence also works for the energy flows along the different processes. Are the heat transport and the ecosystem metabolism connected? This question is not trivial, because even though the dynamical equations look the same, a priori it is not obvious that the thermodynamical expression for the heat transport is exactly the same term in the dynamical equations which corresponds with the ecosystem metabolism rate. Schneider and Kay [179] used experimental data sets for the RB system to plot the total steady state vertical heat transport per unit horizontal area  $W^*$ . (Steady states are denoted with a superscript \*.) Our approach now allows us to write down a simple analytical expression for the heat transport in the steady state, because it will be shown to be related with the total ecosystem metabolism (the total rate of waste production, see (9.40))

$$F_{EM} \equiv (\kappa_{AC} + (1 - q_{CR})g_{CR}C_C)(C_R - C_W^0/K_{eq}) + d_C C_C. \quad (9.22)$$

Our result will suit well the bifurcation behavior as seen in the plot derived by Schneider and Kay<sup>4</sup>.

To calculate  $W^*$ , observe that there is no energy accumulation in the fluid, and hence this heat transport is the same at every height. Therefore it equals the transport at height  $z = 0$ . At the bottom layer, the vertical fluid motion is zero, as is seen in the chosen boundary condition (9.46). Hence, at the bottom layer there is no vertical heat transport by fluid motion. The heat transport is given by the temperature gradient only, as for the conduction state. Taking a horizontal average, the  $Y$ -term in the expansion (9.51) drops out, leaving only

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<sup>4</sup>Schneider and Kay (1994) described a fluid layer with rigid-rigid boundary conditions. Therefore, our results can only be compared qualitatively, as our XZ model only works for systems with free-free boundary conditions.

the  $Z$ -term. This gives:

$$(\rho_0 c_V)^{-1} W^* = -\chi \frac{\partial T^*}{\partial z} \Big|_{z=0} \quad (9.23)$$

$$= \chi \left( \beta + \frac{2\pi Z^*}{h} \right) \quad (9.24)$$

$$= \frac{2h}{\pi^2} \alpha_R (C_R^0 - C_R^*). \quad (9.25)$$

( $\rho_0$  is the reference density and  $c_p$  is the heat capacity.) The latter expression represents the steady state resource exchange  $F_R^*$ , which equals  $F_{EM}^*$  (this is easily seen because there is no accumulation of ecosystem resource or biomass, and hence the net resource exchange should equal the total conversion from resource to waste).

In order to study the behavior of the ecosystem metabolism  $F_{EM}^*$  under different gradients, we need to solve the dynamics for the steady states. Scanning  $\Delta^0$  from zero to infinity, there is a critical value given by the bifurcation point

$$\Delta_c^0 = \frac{(\alpha_R + \kappa_{AC})d_C}{\alpha_R q_{CR} g_{CR}} \quad (9.26)$$

For a value of  $\Delta^0 \leq \Delta_c^0$ , we have only one stable steady state that is physically realistic (no negative concentrations)

$$C_R^* = \frac{\alpha_R \Delta^0}{\alpha_R + \kappa_{AC}} + \frac{C_W^0}{K_{eq}}, \quad (9.27)$$

$$C_C^* = 0. \quad (9.28)$$

Within this region, a stable population of consumers cannot be formed, and hence, only abiotic degradation takes place. However, if the resource input increases so that  $\Delta^0 \geq \Delta_c^0$ , there is the possibility for the consumers to survive at a non-zero concentration. The above state becomes unstable, and the new stable solution is

$$C_R^* = \frac{d_C}{q_{CR} g_{CR}} + \frac{C_W^0}{K_{eq}}, \quad (9.29)$$

$$C_C^* = \frac{q_{CR} g_{CR} \alpha_R \Delta^0 - (\alpha_R + \kappa_{AC})d_C}{d_C g_{CR}} = \frac{q_{CR} \alpha_R}{d_C} (\Delta^0 - \Delta_c^0). \quad (9.30)$$

Using these solutions, the steady state ecosystem metabolism can be written as

$$F_{EM}^* = \frac{\alpha_R \kappa_{AC}}{\alpha_R + \kappa_{AC}} \Delta^0 + \frac{\alpha_R^2}{\alpha_R + \kappa_{AC}} (\Delta^0 - \Delta_c^0), \quad (9.31)$$

where we can clearly see the correspondence from conduction (the first term) and convection (the second term). Fig. 9.4 plots  $F_{EM}^*$  as a function of the thermodynamic gradient  $\Delta^0$ . The (qualitative) similarity with the figure 2a in Schneider and Kay [179] is obvious. The steady states which have only abiotic conversion are located at the so called thermodynamic branch, because this branch contains thermodynamic equilibrium at zero gradient ( $F_{EM}^* = 0$  at  $\Delta^0 =$

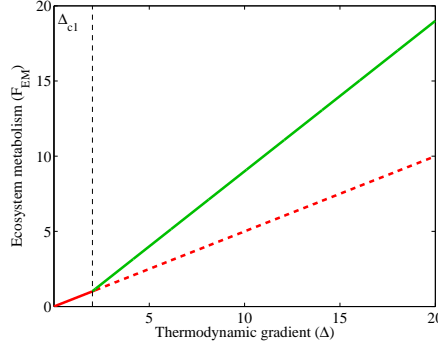


Figure 9.4: The total steady state ecosystem metabolism  $F_{EM}^*$  in function of the driving force  $\Delta^0$ , for specific parameter values. Red color denotes abiotic conversion only, the green line corresponds with biotic consumption. The dashed line corresponds with unstable states.

0). In the RB system, these states correspond with thermal conduction. But above the bifurcation point, there is an exchange of stability: the states located at the thermodynamic branch become unstable and new stable states arise. These are located at the so called dissipative structure branch, and they contain both abiotic and biotic degradation of resource. Once beyond the bifurcation, a viable consumer population can be established. Translated to the RB system, both conductive and convective heat transport processes appear and a viable 'kinetic energy population' is established.

The above discussion shows the exact correspondence between two terms in the dynamics that describe the energy dissipation: the heat transport and the ecosystem metabolism. However, the argument was restricted to the steady state behavior. We will now give some other arguments to demonstrate that there is not only a formal *mathematical* equivalence of the RC and the XZ models, but that the terms in the dynamical equations correspond also *physically* with the different energetic pathways, Fig. 9.5 (compare with Fig. 9.3). This correspondence of the energetic pathways of both systems is also valid in the transient states of the RC and XZ models.

First let us look at the exchange with the external reservoir (E). The fluid has a heat exchange with the heat reservoir at constant temperature  $T_H^0$ . This exchange is due to heat conduction with coefficient  $\chi$ . The ecosystem has the same functioning: The variable  $C_R$  is in contact with the constant  $C_R^0$  with exchange rate  $\alpha_R$ , explaining the relation (9.15) and (9.25).

Next, let us focus on the energetic pathways within the system. In our resource-consumer ecosystem, we have seen that there are basically three metabolic pathways for the consumption of the resource  $C_R$  (see Table 9.2 in appendix 9.8). These are the three arrows arriving at the waste compartment  $C_W^0$  in the figure.

Also our fluid system has three equivalent heat transport and energy transformation pathways (see e.g. (9.22)) :

- M1: There is heat transport by conduction which is qualitatively given by  $W_{cond} \propto \chi(T_H - T_M^0)/(h/4)$ , and this is indeed proportional with the

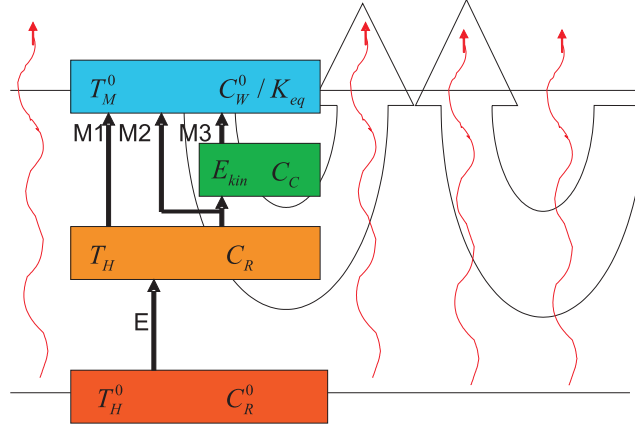


Figure 9.5: The correspondence between temperatures and concentrations, as well as the energetic pathways. The figure shows the lower half of the convective fluid layer, as in Fig. 9.2, with vertical energy transport. The boxes represent the heat energy compartments at three different heights, plus the kinetic energy compartment. In this way, the Rayleigh-Bénard system is presented in terms of a simple resource-consumer food web. See text for more explanations.

abiotic conversion

$$F_{AC} = \kappa_{AC}(C_R - C_W^0/K_{eq}). \quad (9.32)$$

- M2: There is direct heat transport by convection, i.e. heat energy from the lower reservoir is actively transported to the upper reservoir, without being turned in kinetic energy. This is a loss term for the transformation of heat energy to kinetic energy. It is easily seen that this term is proportional with the biotic conversion (which is coupled with the consumer growth, see table 9.2)

$$(1 - q_{CR})F_{RU} = (1 - q_{CR})g_{CR}(C_R - C_W^0/K_{eq})C_C, \quad (9.33)$$

because  $C_C$  is the kinetic energy. Using the dictionary, one can translate this expression into an analytical expression for the direct heat transport by convection  $W_{dir,conv}$ .

- M3: There is heat production due to viscous dissipation of kinetic energy. This extra heat produced is also finally released in the cold temperature reservoir. It is the indirect heat transport by convection, as the heat energy is first turned into kinetic energy, and eventually released again as heat energy. In Kreuzer [89], a derivation is given for this transformation rate of kinetic energy into heat energy:

$$W_{indir,conv} = \frac{\nu}{2} \sum_{\{i,j\}=\{x,z\}} \left( \frac{\partial v_i}{\partial r_j} + \frac{\partial v_j}{\partial r_i} \right)^2,$$

which is indeed proportional with  $\nu X^2$  and hence with biomass decay  $F_{BD} = d_C C_C$  (which in the steady state equals the consumer growth  $q_{CR}F_{BC}$ ).

To summarize, we have demonstrated a unique example of a correspondence between a biological and a physical system. The dynamical equations are equivalent and a dictionary was given between the different quantities. Also the physical interpretations (in terms of energetic pathways) of the different terms in the dynamical equations were proven to be analogous. This correspondence allowed us to calculate an analytical expression for the heat transport in the steady state of the RB system. As Fig. 9.5 shows, a simple resource-consumer food web arises in the fluid system. In the next two sections, we will take this analogy some steps further by expanding the fluid food web in two ways: First we will include competition at the first trophic level (the level of the consumers). Secondly, we will study longer food chains by including predation. In a sense, this approach might allow us to use ecological concepts to extend the Lorenz dynamics in order to find new solutions (i.e. new convection patterns) for the fluid system.

## 9.6 Competitive exclusion and fitness

In ecology, there is the important idea that species can mutate and evolve, leading to Darwinian competition between species. If we describe competition in our ecosystem by taking  $n$  different consumer species with growth rates  $g_{CRi}$ , death rates  $d_{Ci}$  and yields  $q_{CRi}$ , with  $i = 1, \dots, n$ , we can calculate the stable steady state and it appears that the species with the highest value of the competitive fitness

$$f_i \equiv \frac{q_{CRi}g_{CRi}}{d_{Ci}} \quad (9.34)$$

survives, the others go extinct. This is a version of the famous competitive exclusion principle [7].

As pointed out by Nicolis and Prigogine [134], in the fluid at the onset of convection, fluctuations in the form of convection cells appear. These cells or rolls can have different sizes, parametrized by the geometric factor  $a$ . Solving the Lorenz dynamics does not allow us to calculate the size of the convection rolls, because  $a$  is treated as a constant parameter. But as the monoculture resource-consumer ecosystem can be generalized to a polyculture resource-consumers ecosystem, it is tempting to perform a translation in order to construct a generalization of the simplified Lorenz system. This adds a new element in the fluid systems: Rolls with different sizes (different  $a_i$ ) will go into competition with each other.

With this generalization, one can now ask which kind of convection cells are the most fittest, which species of rolls will eventually survive. As the competitive exclusion principle states, the rolls with the highest fitness  $f_i$  will survive, so the only thing we need to do is to translate the competitive fitness measure  $f_i$  to the fluid system and write it as a function of the parameter  $a_i$ . If we do the translation with the above dictionary (9.10-9.16), we get the fluid fitness for rolls with parameter  $a_i$ :

$$f_i \rightarrow \frac{a_i^2 h^3 g \alpha}{(a_i^2 + 1)^3 \pi^3 \nu \chi} \quad (9.35)$$

Note that the geometric factor (9.20) appears in the fitness. There is a trade-off between small and large sizes, and the fitness (9.35) is maximal for rolls with

parameter  $a_i = 1/\sqrt{2}$ , and hence with width  $h/a_i = \sqrt{2}h$ . As was first shown by Rayleigh (1916) using a totally different line of reasoning, this is also the experimentally verified size of the convection rolls at the onset of convection. Furthermore, using this value for  $a$  together with (9.26) and the definition of the Rayleigh number (9.18), we can calculate the critical Rayleigh number  $Ra_c = 27\pi^4/4$ . This is indeed the correct value for the fluid system with free-free boundary conditions<sup>5</sup>.

## 9.7 Conclusions and further discussions

We have seen that one can simplify the dynamical equations of a convective fluid system into a set of two ordinary differential equations which look exactly the same as a simplified resource-consumer ecosystem. Furthermore, there is not only a mathematical correspondence in the structure of the equations, but more remarkable, there is also a correspondence between physical interpretations. This correspondence was then broadened to include competition and predation. With these extensions, we have proven or conjectured more connections. We have translated quantities, processes, energetic pathways,... from fluid systems to ecological systems and vice versa, and we were able to calculate the correct value of the size of convection cells with the help of biological competition and fitness (the competitive exclusion principle from ecology).

Table 11.3 presents the dictionary of the correspondence which is a quantitative extension of the bare essentials given in table 9.1. There is always unstructured gradient degradation, but above a critical level of the gradient, ordered patterns or structures appear: living cells and convection cells.

This striking analogy that we have found between two systems that are at first sight totally different, can be casted in the (more general but often vague) language of dissipative structures (see chapter 8) used by Prigogine and co-workers [65, 134]. Prigogine and co-workers performed quantitative studies of biological systems, but these were mostly restricted to the subcellular level. Schneider and Kay [179] took the correspondence further to the ecosystem level, but their discussion was only qualitative, using often vague words. The discovery of the correspondence between convection cells (a primary example of dissipative structures) and consumer species, together with the discussion in chapter 8, now lead us to the conclusion that the resource-consumer model as described in this chapter is a system that contains dissipative structures.

## 9.8 Appendix: The RCW ecosystem

The resource-consumer-waste ecosystem consists of two environmental reservoirs, one for the resource and one for the waste. As an example, we can think of a chemotrophic ecosystem with glucose or methane as resource and  $CO_2$  as waste product. The resource is supplied from the environmental reservoir at a fixed concentration  $C_R^0$  using a linear exchange mechanism with rate constant  $\alpha_R$  and flux

$$F_R = \alpha_R(C_R^0 - C_R). \quad (9.36)$$

---

<sup>5</sup>This result is non-trivial, as the final words of appendix 9.9 point out.

$C_R(t)$  is the variable resource concentration in the ecosystem. The ecosystem metabolism is the total conversion (degradation) of resource into waste. In our chemotrophic ecosystem, this conversion is an oxidation process. Table 9.2 shows the three metabolic transformations that occur within the ecosystem, together with the kinetic expressions used.

Abiotic conversion	$R \rightarrow W$	$F_{AC} = \kappa_{AC} \left( C_R - \frac{C_W^0}{K_{eq}} \right)$
Resource uptake by biomass synthesis and biotic conversion	$R \rightarrow q_{CR}C + (1 - q_{CR})W$	$F_{RU} = g_{CR}C_C \left( C_R - \frac{C_W^0}{K_{eq}} \right)$ $F_{BS} = q_{CR}F_{RU}$ $F_{BC} = (1 - q_{CR})F_{RU}$
Biomass decay	$C \rightarrow W$	$F_{BD} = d_C C_C$

Table 9.2: Ecosystem transformations

The abiotic conversion is a chemical reaction with equilibrium constant  $K_{eq}$  and a constant abiotic conversion rate parameter  $\kappa_{AC}$ . The latter abiotic conversion rate is increased due to a parallel biotic conversion, described by a simple linear functional response with parameter  $g_{CR}$ . This biotic conversion has two parts: a fraction of the resource is used for consumer growth, the other part of the resource turns immediately into waste. From a thermodynamic perspective, the latter resource turnover is necessary to drive the growth process. This fractioning is described by the yield parameter  $q_{CR} < 1$ : this is the growth efficiency which denotes the amount of resource required to build up one unit of biomass. The third metabolic transformation is the biotic decay (basal maintenance<sup>6</sup>), represented by the rate constant  $d_C$ .

When the resource is turned into waste, the latter is emitted into the waste reservoir from the environment. This environment has a constant waste concentration  $C_W^0$  and the exchange flux can be described as

$$F_W = \alpha_W (C_W - C_W^0). \quad (9.37)$$

Putting the two exchange fluxes and the three metabolic fluxes together, the complete dynamics for the resource concentration  $C_R(t)$ , the consumer biomass concentration  $C_C(t)$  and the waste concentration  $C_W(t)$  now look like

$$\frac{d}{dt}C_R = \alpha_R(C_R^0 - C_R) - (\kappa_{AC} + g_{CR}C_C)(C_R - C_W/K_{eq}), \quad (9.38)$$

$$\frac{d}{dt}C_C = q_{CR}g_{CR}(C_R - C_W/K_{eq})C_C - d_C C_C, \quad (9.39)$$

$$\begin{aligned} \frac{d}{dt}C_W &= \alpha_W(C_W^0 - C_W) + (\kappa_{AC} + (1 - q_{CR})g_{CR}C_C)(C_R - C_W/K_{eq}) \\ &\quad + d_C C_C. \end{aligned} \quad (9.40)$$

This is the RCW model. Next, we have to simplify this model to the RC model, by assuming  $\alpha_W$  to be very large. This means that the relaxation time of the waste exchange is negligibly small, and we get the condition that  $C_W \approx C_W^0$ , resulting into (9.6-9.7).

<sup>6</sup>This biomass decay is due to basal maintenance, as in (4.14) with  $r_C = 1$ . There is no biomass recycling as in chapter 3.

## 9.9 Appendix: The XYZ Lorenz system

In this appendix, we will give all approximations and a schematic derivation in order to arrive at the Lorenz system for the Rayleigh-Bénard convective fluid (see [18, 97]).

In order to present the field equations we will first list the Boussinesq approximations (see e.g. [63]):

- There are no pressure terms in the energy balance equation.
- The heat conduction coefficient  $\chi$  and the kinetic viscosity  $\nu$  are constants.
- The local density field  $\rho$  depends on the temperature as  $\rho = \rho_0(1 - \alpha(T - T_0))$  with  $\rho_0$  and  $T_0$  the constant reference density and temperature,  $T$  the local temperature field, and  $\alpha$  the constant thermal expansion coefficient.
- The above dependence of the density on the temperature is taken into account only in the gravitational force term in the momentum balance equation. At other places in the equations, we will write the density as  $\rho_0$ .
- The fluid is incompressible (except in the thermal expansion term):  $\frac{d\rho}{dt} = 0$ , which results in an equality between heat capacities at constant pressure and volume:  $c_p = c_v$ , or it can be written in terms of the velocity field  $\vec{v}$  as:

$$\vec{\nabla} \cdot \vec{v} = 0, \quad (9.41)$$

- The local internal energy differential is  $dU = c_p dT$ .

With these approximations, the heat transport equation can be derived from an energy balance equation, and looks like

$$\frac{\partial T}{\partial t} = -(\vec{v} \cdot \vec{\nabla})T + \chi \Delta T. \quad (9.42)$$

The first term on the right hand side is the advective heat transport term, and the second is the heat conduction term.

The equation for the velocity field is derived from the momentum balance, and results into the Navier-Stokes equation. In the Boussinesq approximation, this leads to

$$\frac{\partial \vec{v}}{\partial t} = -(\vec{v} \cdot \vec{\nabla})\vec{v} - \frac{\vec{\nabla} p}{\rho_0} - g \frac{\rho}{\rho_0} \vec{1}_z + \nu \Delta \vec{v}, \quad (9.43)$$

with  $p$  the pressure field,  $g$  the gravitational acceleration and  $\vec{1}_z$  the unit vector in the vertical z-direction. On the right hand side we see respectively the advection term, the pressure gradient term, the external gravitational acceleration term and the viscous diffusion term.

As a final step, in order to fully describe our system, we need boundary conditions. The boundary condition for the temperature is simply

$$T(z=0) = T_H^0, \quad (9.44)$$

$$T(z=h) = T_C^0. \quad (9.45)$$

For the velocity, we have

$$v_z(z=0) = 0, \quad (9.46)$$

$$v_z(z=h) = 0, \quad (9.47)$$

because there is no fluid flowing out of the layer. This is not enough, and we need another condition on the velocity. We will take free-free boundary conditions to make the description of the solutions easier. This gives

$$\frac{\partial v_x}{\partial z}|_{z=0,h} = 0. \quad (9.48)$$

In summary, we have five partial differential equations: Three from the three velocity components, one from the incompressibility condition and one from the temperature. Our five local variables are the velocity, pressure and temperature fields. Lorenz made some further assumptions in order to turn these five p.d.e.'s into three o.d.e.'s with only three global variables.

Due to (9.41), one can write the velocity field as  $\vec{v} = \vec{\nabla} \times \vec{\psi}$ , with  $\vec{\psi}$  the stream function. We know from experiment that at the onset of convection (near the critical gradient), a convection roll pattern will arise [63]. Suppose that the axis of the rolls are along the horizontal y-direction. Hence, there will be no  $v_y$  component. The simplest way to obtain this is by assuming  $\psi_x = \psi_z = 0$ .

Next, we want to circumvent the pressure field. This can be done by taking the curl of the velocity equation, resulting into:

$$\frac{\partial \nabla^2 \psi_y}{\partial t} = \frac{\partial \psi_y}{\partial z} \frac{\partial \nabla^2 \psi_y}{\partial x} - \frac{\partial \psi_y}{\partial x} \frac{\partial \nabla^2 \psi_y}{\partial z} + \nu \nabla^2 (\nabla^2 \psi_y) + g\alpha \frac{\partial T}{\partial x}. \quad (9.49)$$

As a final step, we will expand the temperature and  $\psi_y$  fields in Fourier modes, taking the boundary conditions into account, and we will retain only three of these modes:

$$\psi_y = X(t) \sin\left(\frac{\pi ax}{h}\right) \sin\left(\frac{\pi z}{h}\right), \quad (9.50)$$

$$T = T_H^0 - \beta z + Y(t) \cos\left(\frac{\pi ax}{h}\right) \sin\left(\frac{\pi z}{h}\right) - Z(t) \sin\left(\frac{2\pi z}{h}\right), \quad (9.51)$$

with the width of the convection cell equal to  $h/a$ . In fig. 9.1, a physical interpretation is given to the variables  $X$ ,  $Y$  and  $Z$ . Plugging these expressions into the above partial differential equations (9.42) and (9.49), and collecting the factors with the same spatial dependence, gives:

$$\frac{dX}{dt} = -\frac{\nu(a^2+1)\pi^2}{h^2}X + \frac{g\alpha ha}{\pi(a^2+1)}Y, \quad (9.52)$$

$$\frac{dY}{dt} = -\frac{2\pi^2 a}{h^2}XZ \cos\left(\frac{2\pi z}{h}\right) - \frac{\chi(a^2+1)\pi^2}{h^2}Y + \frac{\beta\pi a}{h}X, \quad (9.53)$$

$$\frac{dZ}{dt} = \frac{a\pi^2}{2h^2}XY - \frac{\chi 4\pi^2}{h^2}Z, \quad (9.54)$$

As can be seen, the system does not close because there is a  $\cos(2\pi z/h)$  term. A final approximation consists of taking this cosine equal to one.

We finally arrive at the Lorenz equations, which we will call the XYZ model. Next, we have to simplify this XYZ model to the XZ model, by assuming the

pseudo steady state condition for  $Y$  (i.e. taking  $dY/dt = 0$ ), resulting into (9.1-9.2).

We conclude this appendix with an important remark. There are two important approximations for the XZ model. The first is the cancelation of the cosine factor in (9.53). Therefore, solutions of the Lorenz system are not exact solutions of the complete fluid system in the Boussinesq approximation. In this sense, the result of section 9.6 is not trivial, because we arrived at the correct answer for the size of the rolls whereas the underlying dynamics does not give exact solutions.

Our second approximation is the pseudo steady state restriction. This means that the steady states of the XZ system are also steady states of the XYZ model (but as mentioned above, not necessarily of the complete fluid system). In this article we mostly restricted the discussion to the steady states of the XZ model, but one should be cautious to use this model to try to find correct transient solutions for the XYZ or the complete fluid systems. As an example, the XYZ system has chaotic solutions, whereas these chaotic solutions are absent in the XZ model.

## Chapter 10

# Further discussion

The findings in the previous chapter raise a lot of new questions. This final chapter will present some more speculative ideas. How far can we extend the correspondence between the physical fluid system and the ecological system? This can be done in different progressive steps:

- 1) The previous chapter discussed the Lorenz XZ model, which is only an approximation of the XYZ model. Can one turn this XYZ model into an ecological analog?
- 2) The XYZ model only describes straight convective rolls. Other patterns are possible (i.e. zig-zag rolls). Do they have an ecological analog, such as e.g. predation?
- 3) There are not only static patterns. Sometimes, patterns can slowly change. Does this correspond with 'evolution'?
- 4) Ordered patterns occur only in the laminar regime. What about the turbulent regime? Does this correspond with a complex food web? Are there emergent properties at this most complex, 'megascopic' scale?
- 5) And finally, are there similarities between the underlying mechanisms and 'microscopic' processes?

Some parts of the discussion below are highly speculative, with very vague, philosophical formulations which are difficult to falsify. However, this should not blind the reader for other ideas that are better suited for testing.

### 10.1 From the Lorenz model to a biological model

In the previous chapter we saw an intriguing correspondence between two systems. There were two restrictions we are now going to extend. First, we took the  $Y$ -variable in the steady state before making the correspondence. Secondly, the ecosystem was required to obey  $\alpha_R = \kappa_{AC}$ . We are now going to extend these two restriction, making the analogy between the full Lorenz model and a biological cell growth model.

The Lorenz XYZ model has dynamics (see appendix of chapter 9):

$$\frac{dX}{dt} = -\frac{\nu(a^2+1)\pi^2}{h^2}X + \frac{g\alpha ha}{\pi(a^2+1)}Y, \quad (10.1)$$

$$\frac{dY}{dt} = -\frac{2\pi^2 a}{h^2}XZ - \frac{\chi(a^2+1)\pi^2}{h^2}Y + \frac{\Delta_F \pi a}{h^2}X, \quad (10.2)$$

$$\frac{dZ}{dt} = \frac{a\pi^2}{2h^2}XY - \frac{\chi 4\pi^2}{h^2}Z, \quad (10.3)$$

We now need a lot of redefinitions and restructuring. First, write

$$Y \equiv AX \quad (10.4)$$

and

$$Z \equiv \frac{\Delta_F (\alpha_R(C_R^0 - C_R) - \kappa(C_R - C_R^{eq}))}{\zeta \alpha_R \Delta_E} \quad (10.5)$$

with  $\zeta$  an undetermined prefactor and

$$\Delta_E \equiv C_R^0 - C_R^{eq}, \quad (10.6)$$

$$\Delta_F \equiv T_H^0 - T_L^0 \quad (10.7)$$

the environmentally applied thermodynamic gradients of resp. ecosystem and fluid system.

The Z-equation can be rewritten as

$$\frac{dZ}{dt} = -\frac{\Delta_F(\alpha_R + \kappa)}{\zeta \alpha_R \Delta_E} \frac{dC_R}{dt} \quad (10.8)$$

$$= \frac{a\pi^2}{2h^2}X^2A - \frac{4\pi^2\chi\Delta_F}{h^2\zeta\alpha_R\Delta_E} (\alpha_R(C_R^0 - C_R) - \kappa(C_R - C_R^{eq})) \quad (10.9)$$

so

$$\begin{aligned} \frac{dC_R}{dt} &= \frac{4\pi^2\chi}{(\alpha_R + \kappa)h^2} (\alpha_R(C_R^0 - C_R) - \kappa(C_R - C_R^{eq})) \\ &\quad - \frac{\zeta\alpha_R\Delta_E a\pi^2}{2\Delta_F(\alpha_R + \kappa)h^2} X^2A \end{aligned} \quad (10.10)$$

The Y-equation results into a dynamics for  $A$

$$X \frac{dA}{dt} = \frac{dY}{dt} - A \frac{dX}{dt} \quad (10.11)$$

$$\begin{aligned} &= \left[ -\frac{2\pi^2 a}{h^2}XZ - \frac{\chi(a^2+1)\pi^2}{h^2}AX + \frac{\Delta_F \pi a}{h^2}X \right] \\ &\quad - A \left[ -\frac{\nu(a^2+1)\pi^2}{h^2}X + \frac{g\alpha ha}{\pi(a^2+1)}AX \right]. \end{aligned} \quad (10.12)$$

If  $X \neq 0$ , then the  $X$  factor cancels, so

$$\begin{aligned} \frac{dA}{dt} &= \frac{\Delta_F \pi a}{h^2} - \frac{2\pi^2 a}{h^2} \frac{\Delta_F}{\zeta} \frac{(\alpha_R(C_R^0 - C_R) - \kappa(C_R - C_R^{eq}))}{\alpha_R \Delta_E} \\ &\quad - \frac{(\nu + \chi)(a^2+1)\pi^2}{h^2}A - \frac{g\alpha ha}{\pi(a^2+1)}A^2. \end{aligned} \quad (10.13)$$

Taking  $\zeta = 2\pi$ , we obtain

$$\begin{aligned} \frac{dA}{dt} = & \frac{\pi a \Delta_T (\alpha_R + \kappa)}{h^2 \alpha_R \Delta_E} (C_R - C_R^{eq}) \\ & - \frac{(\nu + \chi)(a^2 + 1)\pi^2}{h^2} A - \frac{g\alpha h a}{\pi(a^2 + 1)} A^2. \end{aligned} \quad (10.14)$$

Let us finally rewrite

$$C_A \leftrightarrow (\nu + \chi)A, \quad (10.15)$$

$$C_C \leftrightarrow \frac{X^2}{g\alpha h^3}, \quad (10.16)$$

$$C_R^0 \leftrightarrow T_H^0, \quad (10.17)$$

$$C_R^{eq} \leftrightarrow T_M^0 \equiv \frac{T_H^0 + T_L^0}{2}. \quad (10.18)$$

In this convention, all the quantities on the right hand sides have dimensions of temperature. From the last two relations, we also get  $\Delta_F = 2\Delta_E$ . We will also split the  $\kappa = \xi\kappa + (1 - \xi)\kappa$ , with  $\xi$  some factor. This splitting allows to describe systems with  $\alpha_R \neq \kappa_{AC}$ .<sup>1</sup>

ecosystem	Lorenz system
$\alpha_R + \kappa$	$4\pi^2 \chi / h^2$
$\kappa_{ac}$	$\xi \kappa$
$g_{CR}$	$\alpha_R a \pi^3 g \alpha h / 2 (\alpha_R + \kappa) h^2 (\nu + \chi)$
$g_{AR}$	$(1 - \xi) 4\pi^2 \chi / (\alpha_R + \kappa)$
$q_{AR} g_{AR}$	$(\nu + \chi) 2\pi a (\alpha_R + \kappa) / h^2 \alpha_R$
$q_{CR} g_{CR}$	$2g\alpha h a / \pi(a^2 + 1)(\nu + \chi)$
$d_A$	$(a^2 + 1)\pi^2(\chi + \nu) / h^2$
$m_A$	$g\alpha h a / \pi(a^2 + 1)(\chi + \nu)$
$d_C$	$2\nu(a^2 + 1)\pi^2 / h^2$

Table 10.1: The correspondence for the Lorenz system

Using the transformations in table 10.1, we can write equations (10.10), (10.14) (in terms of  $C_A$ ) and (9.52) (in terms of  $C_C$ ):

$$\frac{dC_R}{dt} = \alpha_R (C_R^0 - C_R) \quad (10.19)$$

$$- \kappa_{ac} (C_R - C_R^{eq}) \quad (10.20)$$

$$- g_{CR} C_C C_A \frac{C_R - C_R^{eq}}{K_R + C_R - C_R^{eq}} \quad (10.21)$$

$$- g_{AR} (C_R - C_R^{eq}) \left( 1 - \frac{C_A}{K_A + C_A} \right) \frac{C_C}{K_C + C_C}, \quad (10.22)$$

$$\frac{dC_A}{dt} = q_{AR} g_{AR} (C_R - C_R^{eq}) \left( 1 - \frac{C_A}{K_A + C_A} \right) \frac{C_C}{K_C + C_C} \quad (10.23)$$

<sup>1</sup>Note that due to this generalization,  $Z$  in (10.5) no longer corresponds with a temperature at height  $h/4$ , as in previous chapter.

$$-d_A C_A - m_A C_A^2, \quad (10.24)$$

$$\frac{dC_C}{dt} = q_{CR} g_{CR} C_C C_A \frac{C_R - C_R^{eq}}{K_R + C_R - C_R^{eq}} \quad (10.25)$$

$$-d_C C_C. \quad (10.26)$$

We obtain the full Lorenz dynamics if we take the half-saturation constants approximately:

$$K_R, K_C \rightarrow 0, \quad (10.27)$$

$$K_A \rightarrow \infty. \quad (10.28)$$

The above dynamics can be interpreted as a system modeling biological cell growth.  $C_R$  is the concentration of the basic resource, which is turned into an additional substrate (e.g. enzymes, ATP) at concentration<sup>2</sup>  $C_A$ . Finally,  $C_C$  is the biomass concentration of the consumer organisms. The terms in the dynamics can be interpreted as:

- (10.19) is the exchange of the resource with its external reservoir
- (10.20) is the abiotic conversion of the resource to the waste at concentration  $C_W^0 = K_{eq} C_R^{eq}$ , with  $K_{eq}$  the equilibrium constant of the chemical reaction.
- (10.21) is the resource depletion due to the growth of the consumer. This term obeys Michaelis-Menten kinetics[185], with half-saturation constant  $K_R$ . The inclusion of the  $-C_R^{eq}$  term indicates that this growth process should stop when the resource is in thermodynamic equilibrium with the waste.
- (10.22) is the resource depletion due to production of the additional substrate  $A$ .
- (10.23) is the production of additional substrate, with efficiency factor  $q_{AC}$ , the 'yield' for the additional substrate. When  $C_A$  is very small, this production is not limited on the additional substrate. But when  $C_A$  is very large, the production gets limited. The origin for such a limitation could be that the additional substrate requires some essential nutrient which is not abundant in the system. The more substrate there is, the more nutrients are bounded, and the less nutrients are free for other substrate production.
- (10.24) is the decay of the additional substrate, which has a linear and a quadratic term.
- (10.25) is the consumer growth, with efficiency (yield)  $q_{CR}$ .
- (10.26) is the consumer decay (biomass turnover).

We conclude that the full Lorenz system can be translated to describe cell growth with an additional substrate which is necessary to drive the growth.

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<sup>2</sup>Although this additional substrate resides usually only intracellular, due to homogenizing our description, this property is not seen in the dynamics

Note that this growth process itself does not deplete the additional substrate. In this sense, ATP is not a good candidate, because ATP molecules are burned in the process of cell growth, and the corresponding term containing  $-C_C C_A \frac{C_R - C_R^{eq}}{K_R + C_R - C_R^{eq}}$  is absent in the dynamics for  $C_A$ . But enzymes might be good candidates. These enzymes can spontaneously decay, and it takes resource energy to produce them.

The following subsections will be more tentative and speculative, as further hypothetical connections are postulated.

## 10.2 Predating fluid motion

In the previous chapter we have discussed the consequences of competition for the fluid system. Besides ecological competition, predation is also highly important. This leads us to a more speculative idea: Is there a possibility for 'predation' in fluid systems?

In chapter 7, we have studied the resource-consumer-predator (RCP) ecosystem<sup>3</sup>. This system has a second critical bifurcation point

$$\Delta_{c2}^0 \equiv \frac{(\alpha_R + \kappa_{AC})}{\alpha_R} \frac{d_C}{q_{CR}g_{CR}} \left(1 + \frac{d_P}{\alpha_R + \kappa_{AC}}\right) \quad (10.29)$$

such that for values  $\Delta \leq \Delta_{c2}$  we get the 'consumer-only' state (9.27-9.30). For values of  $\Delta \geq \Delta_{c2}$ , the consumer-only state become unstable and the new stable state has a non-zero predator concentration (cfr. eq. 7.35).

Moving to the convective fluid system, we have to study convection patterns that appear beyond a second bifurcation point. As shown in the previous chapter, there is a first bifurcation from conduction to straight convection rolls. In the straight rolls situation, there was only velocity in the x- and z-directions, leading to a non-zero kinetic energy for these two directions. This  $E_{kin,xz}$  was shown to be related with the consumer concentration. But for certain systems (depending on e.g. the Prandtl number), due to the appearance of a velocity gradient in these rolls, there might be changes in the surface tension leading to a new instability at a second critical gradient level. This was experimentally as well as numerically shown [38, 63]. At this second bifurcation a new pattern arises, from straight rolls to zig-zag rolls or rolls with traveling waves in the direction of its rotation axis (the y-direction). In these new patterns, there is also a non-zero velocity component  $v_y$  in the y-direction, leading to a non-zero kinetic energy  $E_{kin,y}$ .

This allows us to propose a conjecture. The Lorenz system was derived by simplifying the Navier-Stokes equations in the Boussinesq approximation. By taking the lowest modes in an expansion, and performing an approximation, the Lorenz system was derived in order to study straight convection rolls. The wavy pattern could not be studied with the Lorenz dynamics. The conjecture states that by including another mode (which we will call W), a new variable that describes the motion in the y-direction, a new set of dynamical equations can be

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<sup>3</sup>Chapter 7 discussed a model where the biomass decay equals the biomass recycling, whereas here it is completely given by the basal maintenance. This section only gives a more qualitative description, and hence the difference between recycling and maintenance is of less importance.

given (after performing some approximations to guarantee that the equations are autonomous), the XZW model. And this set of three equations can be translated into the dynamics of a RCP ecosystem.

More specifically, the hypothesis that one can make is that the predator concentration is proportional with the kinetic energy of  $v_y$ . The interpretation is that the waves are behaving as predators feeding on the velocity gradient (or kinetic energy) of the 'consumer prey' rolls, in a similar way as the consumer prey rolls are feeding on the temperature gradient (heat energy).

We did not prove this conjecture at the level of the dynamical equations, but we will only give some (intuitive) arguments.

First, by looking at the advection term in the heat equation (9.42), one can see that there is a coupling between temperature and velocity, and it is this coupling that was proven to be equivalent with the coupling of consumers with the resource in the ecosystem dynamics. Now, by looking at the advection term in the Navier-Stokes equation (9.43), one can see that there is indeed a coupling between different velocity components, so one might expect that this results in an equivalent coupling between predators and consumers in the RCP dynamics.

Second, our conjecture implies that the predator parameters are related to the fluid parameters, in a similar way as in (9.10-9.16). One might intuitively guess that e.g.  $d_P \sim \nu$ . As can be seen in (10.29), a term  $\frac{d_P}{\alpha_R + \kappa_{AC}}$  appears. As this is the ratio of viscosity over conductivity, this term is proportional with the Prandtl number (9.19). The prefactor is dependent on the geometric factor which now includes the wavelength. As shown in e.g. Busse [26], the second critical gradient level increases when the Prandtl number increases. This is consistent with the increasing behavior observed in (10.29).

A third test for this 'predator - kinetic energy' hypothesis is performed by looking at the thermodynamical level. If our conjecture is correct, the total steady state heat transport should be related with the steady state ecosystem metabolism, as in (9.25). Using  $C_R^*$  (cfr. eq. 7.33), the latter can be easily calculated and is presented in Fig. 10.1. We see that for input concentrations above the second bifurcation point, when predation is possible, the stable predator state has always a *lower* ecosystem metabolism rate than the unstable consumer-only state. Looking for example at the behavior of the Nusselt number (the dimensionless number which is proportional with the total heat transport) in the fluid system (Fig. 6 in [26]), we can see that for all studied parameters, the heat transport in the wavy roll state is indeed always lower than in the straight roll state.

Hopefully, one can rigorously proof this correspondence between ecological and fluidal predation. This would allow us to require more analytical expressions instead of using numerical simulations [38]. Furthermore, if this would be possible, we get a new parameter, the wavelength of the zig-zag or wavy pattern which might be related with the parameters  $q_{PC}$ ,  $g_{PC}$  and  $d_P$ . Perhaps it is possible to derive the experimentally correct wavelength (see [157]) again from competition and fitness at the predator level, because the competitive exclusion principle also works at this level [185].

With our work, we extended the program of Schneider and Kay [179] and others by studying quantitatively the (thermodynamic) properties of dissipative structures at the ecosystem level. This lead to a more exact formulation of the correspondence, but also a new feature appeared, something which was not studied by Schneider et al.: the appearance of 'predative dissipative structu-

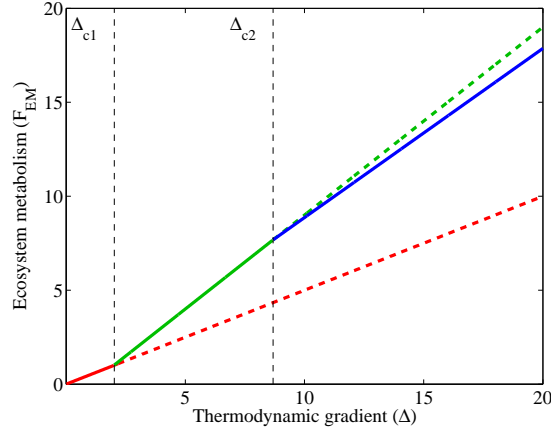


Figure 10.1: The total steady state ecosystem metabolism  $F_{EM}^* = F_R^*$  in function of the external gradient  $\Delta^0$ , for the predator ecosystem. One can clearly see the existence of two critical bifurcation points. Beyond the second bifurcation, the rate in the predator state (blue) is lower than the consumer state (dashed green).

res' after a second bifurcation. Not only is fig. 10.1 an extension of fig. 9.4 (which was shown to be equivalent with fig. 2a in Schneider and Kay [179]), it also shows that the total gradient degradation (by heat transport or ecosystem metabolism) of the consumer-predator state is *lower* than the corresponding unstable consumer state. The predatory dissipative structures make the system less efficient in degrading the thermodynamic gradient.

### 10.3 Convection pattern deformations and ecological evolution

One of the basic problems in convective fluid physics is the pattern selection in the laminar regime [63]. In the previous chapter, we have seen how to answer a pattern selection question about the size of rolls, with the help of ecological concepts, especially competition and fitness. We also conjectured that predation might have a fluid analog, in terms of wavy or zig-zag rolls. Hence, by introducing more species, one can try to gradually move to more complex ecological food webs. By translating them into fluidal terms, one can perhaps study how the different convection cells or patterns behave.

However, as we know from ecology, predator-prey patterns might slowly change due to evolution, and this evolutionary time scale is possibly much larger than the ecological time scale. Do we see the same vastly different time scales in fluid systems? The answer is affirmative, because it is experimentally shown [63] that a convection pattern might slowly change over a time scale of days, which is much larger than the order  $h/v$  with  $h$  the thickness of the layer and  $v$  the typical fluid velocity. The latter time scale can be referred to as the ecological time scale corresponding with the population dynamics, and the former as the longer evolutionary time scale.

Off course, the above affirmation does not prove anything, but at least it adds another analogy to the already many correspondences. Hence, one can ask the (vague) question: Are the unsolved problems in pattern selection perhaps related to some solved or unsolved problems in ecological evolution, and vice versa?

## 10.4 Turbulent fluids and complex food webs

We have seen how predatory structures might arise in fluid systems, due to the appearance of new kinetic energy components. In fluid convection, there are possibly a lot of bifurcations with ever changing patterns of motion. One can try to link this sequence of bifurcations and patterns with a food chain. Adding e.g. a top-predator gives a new, third bifurcation point, and above this point, the ecosystem metabolism in this new state is a bit higher than the unstable predator state. Generalizations to longer trophic cascades are perhaps possible, but finding the analogy with the different kinetic energy components might become difficult to achieve, because the number of independent kinetic energy components is too low. Off course, one can start looking at combinations of kinetic energies, or local variations,... One might also ask the question whether omnivory or more complex food web structures can arise in fluid systems.

This leads us to another hypothesis, by looking at the turbulent regime. Up till now we have been looking at the laminar regime only, and we have seen that there are relations between biological consumers or predators, and different components of the kinetic energy. In the turbulent regime, we can look at the size of whirls or eddies, and more specifically at the (expectation value of the) kinetic energy  $E(k, t)$  at wavenumber  $k$  and time  $t$ . The advantage of this change of perspective is that now we have a very high (infinite) amount of wavelengths, just like we have potentially an infinite amount of possible species in nature.

Let us look at e.g. homogeneous isotropic turbulent systems [197]. The velocity fluctuations of a high Reynolds number (turbulent) flow are typically dispersed over all possible wavelengths. The associated physical metaphor is the Kolmogorov cascade [9], an energy cascade whereby the kinetic energy of large-scale motions (whirls or eddies) is successively subdivided and redistributed among components with increasing wavenumber (smaller and smaller whirls or eddies). The mathematical equation that describes this cascade is

$$\partial E(k, t) / \partial t = F(k, t) - 2\nu k^2 E(k, t). \quad (10.30)$$

The last term is a viscous dissipation term, which is again analogous to the biomass turnover or decay in ecosystems. The  $F(k, t)$  term relates the energies at different wavelengths (it is related to the triple velocity correlation [197]), and this can be interpreted as a prey-predator interaction. The longest wavelengths correspond with basal species of the food web (the species at the lowest trophic level), the shortest wavelengths correspond with top predator species.

This Kolmogorov cascade gives a whole chain of predating fluid currents for the system in a turbulent state, and this corresponds with a potentially very long food-chain or trophic cascade. In ecology, trophic chains have a finite length with a top predator. Also the Kolmogorov cascade has an end member at a finite length scale, the Kolmogorov scale, where viscous dissipation becomes

too strong. Or as Richardson stated: "Big whirls have little whirls that feed on their energy, and little whirls have lesser whirls and so on to viscosity." [165]

In this picture, for example a hurricane can be regarded as a big dissipative structure, with smaller Eddy-current structures predated on it, making up a whole food-chain of structures. Recently there is some evidence for smaller, secondary vortices (e.g. mesocyclones) usually embedded in the eyewall of a hurricane [56]. These smaller vortices might limit the intensity of the hurricane relative to its theoretical maximum intensity it would attain in their absence. Similarly, eddies arising from dynamic instability of the zonal flow in the Hadley cell might limit the strength of the Hadley cell [123]. These limitations in fluid and atmospheric circulations might be comparable to predation losses in food chains.

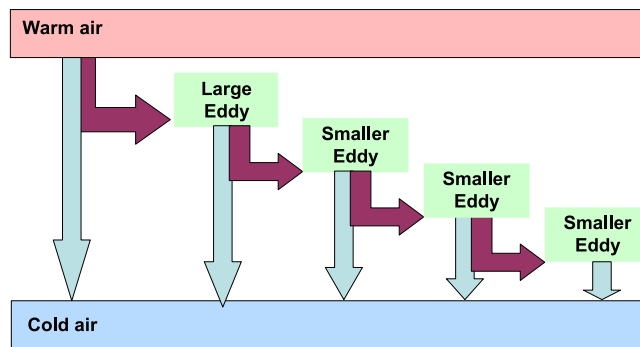


Figure 10.2: The Kolmogorov cascade of a turbulent fluid system.

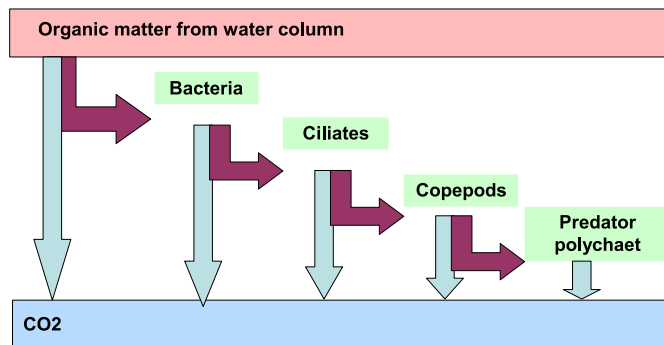


Figure 10.3: The food chain of a marine sediment ecosystem.

So, similar to a trophic chain, turbulence can be seen as a hierarchy of eddies that 'feed' upon the kinetic energy stored in larger eddies. Therefore, a hurricane forms the counterpart of a single trophic compartment, while for example the earth's atmospheric circulation, which shows a spectrum of interacting eddies going from the large Hadley cells to the small Kolmogorov scale, corresponds to a whole food web with its interacting compartments Fig. 10.2 and 10.3 compare the Kolmogorov (turbulent) cascade with the trophic cascade (food chain).

From a fluid dynamics perspective, the one-way picture of the Kolmogorov cascade has been criticised, because direct interactions between large and small

scales can short-circuit the cascade. It is possible to transfer energy from large length scales (big eddies) via smaller length scales to the smallest, but it also becomes possible to directly transfer energy to much smaller scales [9]. Remarkably, such short-circuitry strengthens our analogy, as in ecological parlance, it simply corresponds to omnivory [128]. This way, we can swap the too simple analogy by Schneider and Kay [179] between fluid and ecosystems for a more complex one. Complex food webs might correspond with turbulent systems, turbulent systems might be represented as complex food webs. The advantages of this new perspective on turbulence are that it opens the possibility to achieve long food chains, and that it even might include omnivory as well.

Are the unsolved problems in turbulence related to some solved or unsolved problems in ecological complex food webs, and vice versa? And what is the structure of the 'food web' in turbulent fluids? It is well known that there is a critical level of the external gradient where a transition from laminar to turbulent motion occurs, but the explanation for this curious behavior is still lacking. Laminar convective fluid motion was related with simple food webs. But how to explain the shift towards more complex food webs if the analogy with turbulence would be valid? Characterizing laminar versus turbulent motion might have an analogy in ecology: characterizing simple versus complex food webs. The generalized Lotka-Volterra chemostat models we studied in previous chapters all had a simple food web with a fixed structure. But the structure of real food webs is not rigid, and the question is how to model such evolving, complex food webs realistically. As simple food webs refer to a macroscopic level of ecosystem description, there is a higher scale possible: the megascopic, where high complexity is at work.

## 10.5 The megascopic scale: A new hope for MaxEP?

We finally come back to the partial steady state MaxEP problem, as mentioned in sections 3.6 and 5.5. We have established a rigorous correspondence between simple ecosystems (with a low number of macroscopic variables) and a laminar convective fluid system. Both systems have a low number of different types of dissipative structures that predate and compete with each other. Furthermore, we have conjectured that this correspondence might be extended to the turbulent regime, where a complex food web of multiple dissipative structures interact with each other.

Prime examples of complex turbulent systems are planetary climate systems. And there is some experimental corroboration for a partial steady state MaxEP principle in those systems. Therefore, it is tempting to think that this MaxEP might be valid in highly complex food web ecosystems. In chapter 6 we have seen that a resource-consumer-omnivore system does not obey the partial steady state MaxEP hypothesis. However, one can argue that even though our RCO system is complex and non-linear, it is 'not complex and non-linear enough', it does not have enough degrees of freedom (we have basically only three macroscopic variables:  $C_R$ ,  $C_C$  and  $C_O$ ).

The success of equilibrium thermodynamics was based on a statistical up-scaling (see fig. 10.4), whereby microscopic trajectories become less and less

important when taking the macroscopic limit. In this limit, emergent laws appear, like maximum entropy, Fourier's or the chemical reaction kinetics. Some intuition might indicate that a similar kind of statistical upscaling, a 'law of large numbers' can be applied in non-equilibrium complex systems. The macroscopic system might have dissipative structures in the far-from-equilibrium regime. And perhaps one can take a 'megascopic' limit with multiple types of dissipative structures at multiple length scales. The high amount of different biological cells build up a megascopic ecosystem, and also the high amount of fluid motions and eddies build up a megascopic climate system.

It is not guaranteed that a statistical upscaling is possible. The upscaling from micro- to macroscopic behavior required some special properties (e.g. conservation laws) of the underlying microscopic dynamics. Similar requirements might be absent in the macroscopic dynamics of individual dissipative structures. E.g. relevant conserved quantities might be difficult to find. Therefore, a simple upscaling to the megascopic level will be difficult to achieve. But if the upscaling would be possible, perhaps this might result in an emergent law? And perhaps this law is MaxEP?

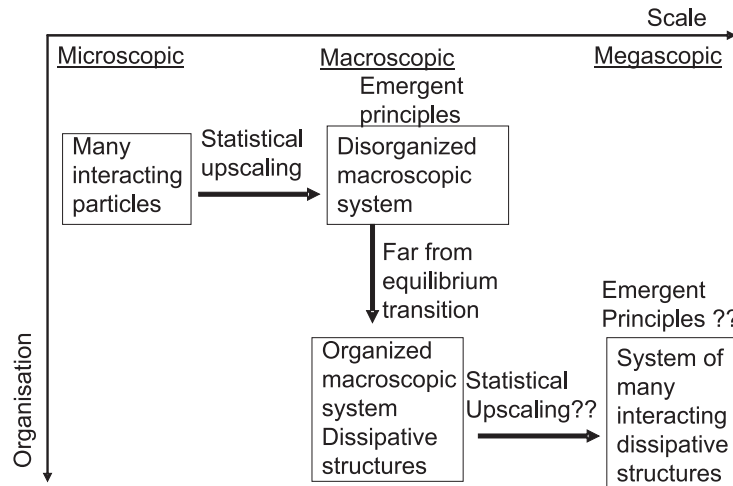


Figure 10.4: The statistical upscaling hypothesis. At the macroscopic level, emergent laws appear from a statistical upscaling of microscopic dynamics. Could it be possible that a similar statistical upscaling at the megascopic scale leads to emergent laws for multiple interacting dissipative structures?

In chapter 3 and section 5.5, we have seen the relevance of the MaxEP hypothesis. For the moment we still have to be sceptical, but perhaps the time is ready to test it in the laboratory. A chemostat ecosystem with a continuous inflow of a resource could serve well. At the theoretical level, to explain the experimental successes of MaxEP in e.g. atmospheric models, one need to know what kind of properties are required for the internal dynamics in order to obtain the MaxEP state.

## 10.6 The microscopic scale and underlying mechanisms

### 10.6.1 Velocity correlations and genetic information

Up till now, we have only looked at the macroscopic or megascopic level. Let us now look at a more microscopic level, which might involve some statistical mechanics and information theory.

We have mentioned the analogy of evolution in a convective fluid system. This analogy might go further: (genetic) mutations are like random microscopic fluctuations, and as noted by Nicolis and Prigogine [134], depending on the environment and the system state, these new fluctuations can be selected and preferred, so they can grow or die out. Also, like the DNA in biotic systems is a memory device with low entropy, the inertia of the momentum of the flows has also a memory content, and the convecting dissipative structure states have a lower entropy than the thermodynamic equilibrium state.

So at the microscopic level, there is information contained in the statistical correlations between the motions of the fluid particles, and perhaps this corresponds with information in DNA and other complex molecules. And when new microscopic fluctuations arise, these correlations change, and hence they might be similar with the changes in DNA due to mutations. When a convection cell is locally formed due to a fluctuation, it reproduces itself due to a viscous dragging of the surrounding fluid, which also starts to move around. In this process, information is transferred from one cell to the other, just as the transfer of DNA information from one cell to the other.

These analogies like the information memory due to correlations, the mutation behavior and the information reproduction, are still highly speculative, and they need much more profound research.

### 10.6.2 Buoyancy force and biological growth

At a less speculative level, we can also look at an hypothetically common underlying mechanism. The crucial element in the existence of convection cells is the buoyancy force. Roughly speaking, the following happens: The heat energy gradient creates a density gradient because the lower, hottest part of the fluid becomes less dense due to thermal expansion. This density gradient results into a state with higher potential energy. When this stored potential energy reaches a critical level, it makes the system unstable, and it is turned into kinetic energy. Finally, the kinetic energy is released as low temperature heat due to viscous dissipation.

In biological cell growth, a similar mechanism works. Starting by a chemical energy gradient (difference in chemical potential), a new 'potential' (also a chemical energy gradient) can be build by creating energy carriers like ATP out of ADP. Having created enough ATP, the cell can start to grow by using this ATP stored energy to build up more biomass. Finally, the biomass is decomposed into waste due to biomass turnover. Hence, we make the hypothesis that the buoyancy mechanism works in the same way as the biological ATP-ADP reactions.

### 10.6.3 Properties of life

All the above ideas are very tempting. They have the potential for the conclusion that a purely physical system can be described in a very similar way as a biological system, and vice versa. This raises rather philosophical questions like 'What is life?' Are fluid cells 'alive'? Giving a definition of life is very difficult. One often encounters at least seven necessary (but vague) criteria to define life. Let us try to apply them to the fluid system.

1) Homeostasis: Regulation of the internal environment to maintain a constant state. We have seen that in the regime with a bacterial monoculture,  $C_R^*$  is constant, independent on the external resource input  $C_R^0$ . So this is a homeostatic effect: Increase the input a bit, and  $C_C$  would settle in such a state that  $C_R^*$  remains the same. Also our convective fluid model shows an analogous homeostatic behavior, because the velocity adapts itself. This self-organizing behavior is due to the large dependence of the dynamics on positive and negative feedbacks.

2) Organization: Being composed of basic units (cells) with high order. Convective cells or eddies are highly organized (as can be seen if one looks at velocity correlations), as are living cells.

3) Metabolism: Converting 'non-living' energy (heat, radiation, chemical resource...) into 'living' energy (kinetic energy, biomass,...), and degrading this 'living' energy into 'non-living' (by viscous dissipation, biomass turnover,...). Living organisms require energy to maintain internal organization (homeostasis) and to produce the other phenomena associated with life. The connection in the previous chapter made it clear that in this way, a fluid system has a 'metabolism'.

4) Growth: Maintenance of a higher rate of synthesis than catalysis. A growing organism increases in size in all of its parts, rather than simply accumulating matter. The particular species begins to multiply and expand as the evolution continues to flourish. Also in convective systems one can see patterns growing. As (auto-)catalytic reactions, this growth is related to the non-linear dynamics.

5) Adaptation: The ability to change over a period of time in response to the environment. As discussed above, also fluid systems can adapt themselves to new temperature, pressure,... gradients. This often gives a (small) change of the convection pattern.

6) Response to stimuli. Disturbing the convective system, the pattern responds by changing into a new pattern. After the disturbance, the pattern might fall back to the previous one.

7) Reproduction: The ability to produce new organisms. Due to the viscous drag at the neighboring fluid, one convection cell 'reproduces' itself. The idea can also be seen in turbulent systems, as a large eddy might split into smaller ones, and the latter can grow by feeding on (heat, kinetic or potential) energy. Presented in this way, it is tempting to look at physical fluid convection as being alive. But the above criteria are still quite vague. At least two major differences between fluid systems and biological systems are:

1) the former usually operate at much smaller time scales (from nano-seconds to days), whereas the latter has a much wider range (from nano-seconds to billion years), and

2) the former are collisions between fluid particles, whereas the latter involve numerous chemical reactions with a lot of chemical elements.

## 10.7 Solving the basic problem in thermodynamic ecology?

Let us finally move back to the basic problem in thermodynamic ecology, which we encountered at different places in this work. It can be summarized by the question: What is the chemical potential of an organisms? This question is related with similar questions about the entropy or the free energy of organisms, as well as the thermodynamic forces for biological processes. Can the correspondence with the fluid system shed some new light on this difficulty?

The driving force for heat flux between different temperatures  $T_1$  and  $T_2$  is given by the difference of the inverse temperatures  $(1/T_2 - 1/T_1)$ . The driving force for the chemical reaction between substances at concentrations  $C_1$  and  $C_2$  is the difference of the chemical potentials  $\mu_2(C_2) - \mu_1(C_1)$ . Therefore, we can relate

$$\mu \sim 1/T, \quad (10.31)$$

at least for the resource and the waste: We have seen that the resource and waste concentrations  $(C_R^{(0)}, C_W^0)$  correspond with the temperatures  $(T_H^{(0)}, T_M^0)$ . The latter are basically equivalent with the internal heat energies. As these internal heat energies have well defined temperatures, the relation (10.31) indicate that the chemical potentials for the resource and the waste should also be well defined for the correspondence to hold.

But what about the chemical potential of the consumer biomass at concentration  $C_C$ , which was shown to be related with the kinetic energy? This chemical potential is not simply related with the inverse temperature of the kinetic energy, as the latter is meaningless. To see what is the correct relationship, we have to look at the part of the EP corresponding with viscous dissipation and biomass decay. The latter has the flux  $F_{BD} = d_C C_C$  and (if it is well defined) the force  $X_{BD} = \mu_C - \mu_W$ , i.e. the difference between chemical potentials of consumer and waste. The EP is  $\sigma_{BD} = F_{BD} X_{BD}$ . On the other hand, the convective fluid system has EP due to viscous dissipation, the turn-over of kinetic energy to heat energy [89]. The EP density of this process is given by

$$\sigma_{visc} = \frac{1}{T} \sum_{i,j} \Pi_{ij} \frac{\partial v_i}{\partial r_j} = \frac{\nu}{2T} \sum_{i,j} \left( \frac{\partial v_i}{\partial r_j} + \frac{\partial v_j}{\partial r_i} \right)^2, \quad (10.32)$$

with  $\nu$  the shear viscosity,  $\Pi$  the viscous pressure tensor,  $r_i$  the position coordinate and  $i$  and  $j$  the velocity directions (for example the  $x$  and  $z$  directions when the axes of the straight roles are along the  $y$  axis). If we would strictly apply the correspondence, we have to look for a relation between  $\sigma_{BD}$  and  $\sigma_{visc}$ , and this might give a hint for the determination of  $\mu_C$ . However, such a relation is not (yet) clearly visible. And even if  $\mu_C$  could be translated into fluid terms, this does not give a hint about the functional relation  $\mu_C(C_C)$ , in the same way that  $\mu_R \sim 1/T_H$  does not indicate that  $\mu_R \propto \ln C_R$ . Using the correspondence between fluid and ecosystems to calculate the chemical potential of the consumers might be an interesting strategy, but it is very doubtful whether the correspondence can be stretched out that far. For the moment it remains an open avenue which we shall leave for future research.

## 10.8 The state of the field: Where do we stand?

*What is the current state of the field, and what is the contribution from our work?*

The physics of non-equilibrium systems, as well as the thermodynamics of ecosystems is plagued with a large amount of fuzzy words: ordered, complexity, dissipative structures, gradient dissipation, goal functions,... With these words, one can encounter a lot of statements and hypotheses in the literature. But how to test these theories when there is only a vague description and no quantitative setting? So we improved some discussions by defining goal functions and dissipative structures and by classifying EP principles and hypotheses. These descriptions lend themselves for theoretical modeling. A lot of hypotheses and assertions were refuted by calculating properties (such as the entropy production) for very simple ecosystem models.

However, our models were very restricted. They describe a macroscopic setting of ecosystems, which means that the structure of the food web was fixed. When food webs can change and evolve, highly complex ecosystems might develop. One can take two opposite expectations towards this increased level of complexity (the megascopic level). The first, pessimistic point of view states that it was a very simple job to find counter examples, that nothing guarantees that the hypothesis holds at the megascopic level. On the other hand, the optimist claims that complexity comes to the rescue. So the next job is to study some hypotheses, especially MaxEP (see chapter 3), for highly complex self-organizing systems with some emergent behavior. These hypotheses are also in high need for testing, either by experiments or by field observations. Our description of chemotrophic ecosystem models can be applied to e.g. laboratory chemostats or oceanic sediments, because the crucial quantities (the net inflow of resource and the chemical potentials of resource and waste substrates) can be rather easily measured.

But our study to look for thermodynamic goal functions in ecosystems and its relation with thermodynamic properties of dissipative structures also led us to another discovery: There is an analogy between climate systems and highly complex megascopic ecosystems, and there is an even stronger analogy between laminar convective fluid systems and macroscopic ecosystems with simple food webs. The former analogy might shed some new light on the MaxEP hypothesis, as well as turbulent fluid motions. The latter analogy might be applied to study e.g. pattern selection problems in convective fluid layers. There are also intriguing questions related with a more microscopic approach of self-organization (by information replication) in fluid and ecosystems. Up till now, we were not yet able to derive new non-trivial results, because solved problems were related with solved ones, and unsolved with unsolved ones. We hope that besides the aesthetically pleasing results we have found, one is able to use the analogy to find new solutions to important problems, both in ecology and fluid physics.

## Chapter 11

# Summary of most important results

Let us briefly summarize the most important results of this thesis. As the subtitle "Entropy production and the analogy between fluid, climate and ecosystems" suggests, there are two aspects: the EP and the analogy.

### 11.0.1 Entropy production

We have derived a reliable expression for the total EP of chemotrophic ecosystems in the steady state:

$$\sigma_{tot}^* = \alpha_R(C_R^0 - C_R^*)R \ln(K_{eq}C_R^0/C_W^0), \quad (11.1)$$

with  $\alpha_R$  the resource exchange rate,  $C_R^0$  the environmental resource concentration,  $C_R^*$  the steady state ecosystem resource concentration,  $R$  the gas constant,  $K_{eq}$  the chemical equilibrium constant for the resource-waste reaction and  $C_W^0$  the environmental waste concentration.

Studying this EP for a resource-consumer-omnivore system with resource exchange limitation, we have obtained the following conclusions:

- The selected steady state is *not* always the one with highest EP,
- the EP does *not* always increase under evolution,
- the EP of the living state is *not* always higher than the corresponding dead state and
- the EP does *not* always increase when the system is driven further out of equilibrium.

### 11.0.2 Analogy

Table 11.1 summarizes the analogy at three levels of description for the fluid (climate) and the ecosystem. The correspondence is quite strongly established at the macroscopic level, with some remaining open problems. But especially the micro- and megascopic levels have much unsolved questions in need for clarification and further scrutiny.

Level	Micro (???)	Macro (?)	Mega (???)
Fluid system	Velocity correlations	Laminar convection cells	Large systems (climate) or turbulent motion
Ecological system	Molecular information	Simple, static foodweb	Large, flexible, complex foodweb

Table 11.1: The correspondence at three levels of description. The more question marks, the more speculative the correspondence: Especially the micro- and megascopic scale are very preliminary and problematic.

### Megascopic level

At the megascopic level, there is an analogy between climate modeling and ecosystem modeling. The effective ecosystem dynamics contains only resource and waste as variables, as the ecosystem itself is treated as a black box. The basic equations are

$$\frac{dC_R}{dt} = \alpha_R(C_R^0 - C_R) - \kappa_{EM}^\times(C_R - C_W/K_{eq}), \quad (11.2)$$

$$\frac{dC_W}{dt} = \kappa_{EM}^\times(C_R - C_W/K_{eq}) - \alpha_W(C_W - C_W^0), \quad (11.3)$$

with  $C_W$  the ecosystem waste concentration,  $\kappa_{EM}^\times$  the effective ecosystem metabolism rate and  $\alpha_W$  the waste exchange rate. The following table translates this system into a planetary climate system with heat transport between the tropics and the poles as the only two heat compartments.

	climate system	ecosystem
max. tropic temperature	$T_T^0$	$C_R^0$
min. pole temperature	$T_P^0$	$C_W^0/K_{eq}$
average tropic temp.	$T_T$	$C_R$
average pole temp.	$T_P$	$C_W/K_{eq}$
relaxation rates	$\alpha_T, \alpha_P$	$\alpha_R, \alpha_W$
effective atmospheric heat transport rate	$\kappa_A^\times$	$\kappa_{EM}^\times$

Table 11.2: The correspondence between the parameters and variables of the climate and ecosystem.

Some planetary observations indicate that  $\kappa_A^\times$  is close to the value whereby the atmospheric EP is at a maximum [148]. This might indicate an emergent property, whereby a very large amount of possible atmospheric (and oceanic) fluid motions, from small clouds and whirls to large hurricanes and Hadley cells, operate together to maximize the EP. The hypothesis is that  $\kappa_{EM}^\times$  might also be close to the value whereby the ecosystem metabolism has a maximum EP. This might indicate an ecological emergent property whereby a large amount of organisms, species and processes might collectively result in a maximum metabolic EP. For the moment, clear experimental observations that verify the hypothesis are still missing.

The megascopic scale of a fluid might also refer to the complexity of turbulent fluid motion. The hypothesis is that turbulent fluid motion has energy transfers along different eddies, forming a complex food web. The Kolmogorov cascades in turbulent systems might correspond with trophic chains in ecosystems.

### Macroscopic level

At the macroscopic level, there is an analogy between a fluid system in the laminar convection regime and an ecosystem with one resource and a few species (consumers and predators). The resource-consumer dynamics looks like:

$$\frac{d}{dt}C_R = \alpha_R(C_R^0 - C_R) - (\kappa_{AC} + g_{CR}C_C)(C_R - C_W^0/K_{eq}), \quad (11.4)$$

$$\frac{d}{dt}C_C = q_{CR}g_{CR}(C_R - C_W^0/K_{eq})C_C - d_C C_C, \quad (11.5)$$

with  $C_C$  the consumer concentration,  $\kappa_{AC}$  the abiotic conversion (from resource to waste) rate parameter,  $g_{CR}$  the consumer growth rate parameter,  $q_{CR}$  the yield factor for the consumer growth and  $d_C$  the consumer decay rate parameter. Table 11.3 translates this ecosystem dynamics to a model that describes the Rayleigh-Bénard fluid system, a horizontal fluid layer heated from below<sup>1</sup>.

	fluid system	ecosystem
Temperature at lower part <sup>2</sup>	$T_H$	$C_R$
Temperature at bottom	$T_H^0$	$C_R^0$
Temperature at middle (axis) of convection cell	$T_M^0$	$C_W^0/K_{eq}$
kinetic energy	$X^2/g\alpha h^3 (\propto E_{kin})$	$C_C$
growth (buoyancy)	$g\alpha h a^2 \pi^2 / (a^2 + 1) \chi$	$g_{CR}$
yield	$8/\pi^4 (1 + a^2)$	$q_{CR}$
decay (viscosity)	$2\pi^2 (a^2 + 1) \nu / h^2$	$d_C$
heat inflow	$2\pi^2 \chi / h^2$	$\alpha_R$
heat conduction	$2\pi^2 \chi / h^2$	$\kappa_{AC}$
fitness	$g\alpha h^3 a^2 / \nu \chi \pi^3 (a^2 + 1)^3$	$q_{CR}g_{CR}/d_C$

Table 11.3: The translation from the ecosystem to the laminar convective fluid system. It indicates that biomass corresponds with kinetic energy, abiotic resource conversion with heat conduction and biotic conversion with convection.

### Microscopic level

At the microscopic level, there might be a similarity in the underlying mechanisms that result into the macroscopic self-organizing behavior of fluid motions and ecosystems. Macroscopic fluid motion requires a microscopic correlation of the velocities of the fluid particles. Viscous drag might transfer the information content of these correlations from one fluid whirl to another. Similarly, DNA contains genetic information that is transferred in the process of cell division.

<sup>1</sup> $h$  is the thickness of the layer,  $X$  is the maximal velocity of the convection cell,  $g$  is the gravitational acceleration,  $\alpha$  the thermal expansion coefficient,  $a$  is height/width,  $\chi$  is the heat conduction coefficient and  $\nu$  is the kinematic viscosity

## Chapter 12

# Endnote and personal confession

Some ecosystems have a gradual succession to a climax state. Starting from a deserted or highly degraded landscape, first pioneer plants arrive. They prepare for better living conditions for other plants by fixing nutrients, increasing the water-holding capacity,... As new immigrants arrive, they benefit from the preparations by the pioneers. After a while, the pioneers are often outcompeted and the second stage sets in. This process might go on, and after several stages, an optimal 'climax' state might be reached, e.g. a full grown forest.

The evolution in thermodynamic ecology is similar. As in ecosystems, with trial and error new challenging ideas clear the path for further research and development. But sooner or later those pioneer proposals are competed out by other ideas and the second stage sets in. This thesis tells us the story about the evolution towards this second stage: there is a deep analogy between two types of dissipative systems, a convective fluid system and an ecosystem. The dynamical equations are the same, as well as a number of physical properties. This opens up a new research program, as a lot of new challenging ideas are proposed in the previous chapters. Sooner or later, our ideas will be challenged, and a third stage might set in. One step up, all the way to the climax.

Let me end with a personal confession. Thermodynamic ecology is a new and interdisciplinary research, it suffers some childhood diseases. Better communication between both fields of science, between physics and ecology, is required. These fields have subtle differences in language and vision, so it was a challenge for a theoretical physicist to talk and collaborate with ecologists. As it is a new branch in science, it is subject to some dangers. Concepts of one field might be applied too carelessly to the other field. The hope to find new 'universal unifying laws' should not paralyze critical thinking. In this thesis, a lot of criticism on other studies was given. And it is only a small fraction... When I delved deeper into the subject, a shocking experience came to me. From all the books and articles listed in the bibliography, I can give (mostly substantial) negative comments on nearly the half(!) of them. Only one quarter of the citations are scientifically satisfying in my personal opinion, and roughly one quarter are undecided. This does not mean that I consider these negatively commented stu-

dies to be worthless, as they are the pioneering plants that prepared the way. But caution is needed in this interdisciplinary branch of science. True science tries to test and falsify proposals. Therefore, I challenge both physicists and ecologists to test the ideas from the previous two chapters, and to move to the third step. Let us hope that sooner or later we will reach the climax state of a 'universal, unifying law'...<sup>1</sup>

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<sup>1</sup>But... at the long evolutionary (geological) timescale, also climax states will be disrupted... We never know the end.

# Appendix A

## Glossary

*Anabolism*: The energy demanding synthesis of complex molecules out of elementary molecules.

*Autotroph*: An organism that produces complex organic compounds from simple inorganic molecules (e.g.  $CO_2, \dots$ ).

*Attractor*: A notion in non-linear physics to denote a set to which a dynamical system evolves. They can be classified into fixed points (steady states), limit cycles (periodic states), limit tori (quasiperiodic states) and strange attractors (chaotic states).

*Biotic conversion*: Direct conversion of resource to waste which is associated with the growth process. This conversion process is energetically coupled with the biomass synthesis. It represents the 'energetic cost' due to *active maintenance* of the growth. The biotic conversion is 'direct' in the sense that the resource is not first transformed into e.g. biomass that eventually decays into waste. For a consumer feeding on the resource, the biotic conversion is synonym with the resource *catabolism*.

*Biomass synthesis*: Production of biomass out of resource compounds. Synonyms: *anabolism*, *biomass assimilation*.

*Biomass decay*: The decay of biomass into resource compounds (*biomass recycling*, *biomass turn-over*) or waste products (*basal maintenance*).

*Catabolism*: The energy releasing breakdown of large molecules into smaller units.

*Chemotroph*: An organism that obtains energy by the oxidation of electron donating molecules in their environments.

*Chemotrophic ecosystem*: An ecosystem whereby all organisms are chemotrophic. There are two types of chemotrophic ecosystems. Chemoheterotrophic ecosystems are systems whereby the organisms are feeding on (dead) organic matter, for example sediment ecosystems at the bottom of an ocean or lake.

(Dead) *organic* chemical compounds (which are in reduced state), like glucose  $C_6H_{12}O_6$ , fall on the sediment surface and serve as food resource with high energetic quality. This resource is turned into waste products, like  $CO_2$ , which is in oxidized state and has a low energetic quality. Chemoautotrophic systems contain organisms feeding on an abiotic energy substrate and synthesizing organic compounds from  $CO_2$ , for example marine hydrothermal vent systems, where *inorganic* chemical compounds with high energetic quality (e.g.  $H_2S$ ) percolate out of the sea floor, and these reduced chemicals are then oxidized to e.g.  $SO_4$  with low energetic quality. These chemical oxidation reactions drive the biological processes.

*Compartment*: A graphical representation of a specific type of particle or species at a specific place. E.g. the carbon atoms in a tiger population in place A, the carbon atoms of a rabbit population in place B, the carbon atoms in detritus in place C, are different examples of compartments. Fluxes between compartments form a network, such as a food web.

*Ecosystem ecology*: The study of the flows of energy and matter through the biotic and abiotic components of ecosystems.

*Ecosystem metabolism*: The total production of waste (products with low energetic quality). This consists of the sum of abiotic conversion, biotic conversion and (when present) the direct decay of biomass into waste products (due to basal maintenance).

*Eddy*: the swirling of a fluid, e.g. as it flows past an obstacle. Synonyms: *vortex**vortex*, whirl.

*Environment*: The part of the model universe that does not contain the ecosystem. In theoretical modeling, the environment is described by *environmental reservoirs*: compartments in internal equilibrium and with very large relaxation times (e.g. by taking very large volumes, heat capacities) such that intensive quantities are approximately constant. The environment is (far) away from equilibrium when the intensive quantities of different reservoirs are (highly) different.

*Equilibrium*: (Thermodynamic-) The state of a thermodynamic system which is in thermal, mechanical (the sum of the forces, and torque, at each part of the system is zero), and chemical (the concentrations of the reactants and products have no net change over time) equilibrium. This means that the temperatures, pressures and chemical potentials of all components are the identical, homogeneous and constant. Synonym: *global equilibrium*. See also near equilibrium, far from equilibrium, local equilibrium.

*Extremal principle*: The general name for a principle or hypothesis whereby a quantity (e.g. a functional or a function) attains a maximum or a minimum (in some general sense). Extremal principles can be classified in different ways. A *variational principle* uses a differentiable quantity, and the extremum is obtained by variation. A *non-variational principle* is a selection principle out of a discrete set of possibilities (e.g. steady states). Another classification makes the distinction between a *transient state extremal principle* to derive equations of

motion, and an *attractor state extremal principle* to find the attractor state(s). A third possible distinction is between *Lyapunov* and *non-Lyapunov principles* (see Lyapunov function). *Organizational principles* in non-linear systems are often extremal principles. Synonym: *goal function principle*.

*Far from equilibrium*: Not close to equilibrium. If the far from equilibrium system is still in local equilibrium (which is not necessary), the forces can no longer be approximated to be linear functions of the fluxes.

*Heterotroph*: An organism that requires organic substrates to get its carbon for growth and development.

*Local equilibrium*: The intensive thermodynamic quantities (temperature, pressure, chemical potential) are space and time dependent, but they are varying so slowly that for any point, one can assume thermodynamic equilibrium in some neighborhood around that point. When the variations of the intensive quantities become too large, the very assumptions (e.g. the thermodynamic limit, the statistical law of large numbers) upon which the definitions of these quantities are based will break down, and the system will be in neither global nor local equilibrium.

*Lyapunov function*: A scalar function  $L(x)$  from the phase space  $\mathbf{R}^n$  to  $\mathbf{R}$ , which is

- positive definite on a neighbourhood region  $D$  around  $x^*$ :  $L(x^*) = 0$  and  $L(x \in D \setminus \{x^*\}) > 0$ , and
- $\dot{L}(x) \leq 0$  on every trajectory in  $D$  obeying  $\dot{x} = f(x)$ , with  $f(x^*) = 0$ .

The existence of a Lyapunov function guarantees that  $x^*$  is a stable steady state under the dynamics  $\dot{x} = f(x)$ .

*Near equilibrium*: A system in local equilibrium whereby the thermodynamic forces are small such that they are approximately linear in the conjugate fluxes. Synonym: linear response regime, close to equilibrium.

*Phototroph*: An organism that obtains energy from light radiation. It carries out photosynthesis.

*Phototrophic ecosystem*: An ecosystem whereby some organisms (the primary producers) are phototrophic.

*Resource uptake*: The transformation of resource into biomass (biomass synthesis) or waste products (biotic conversion), due to the biological growth process. The sum of biomass synthesis and biotic conversion.

*Thermodynamic gradient*: A suitable measure for the distance from equilibrium, in appropriate units. It is typically the difference of concentrations or intensive quantities (e.g. temperatures) of two compartments. The gradient is related with the *thermodynamic driving force*, but the latter often has inappropriate units (e.g. Joule/Kelvin instead of mole or Kelvin) or more complex dependence

on the variables that appear in the dynamics (e.g. logarithms of the concentrations, inverse temperatures) and therefore becomes less suitable for modeling.

## Appendix B

# Notational conventions

We have tried to keep the notation as uniform and self-explaining as possible. Let us summarize the most important quantities and rules.

superscripts: time-constant quantities

environment: superscript 0

quasi steady state: superscript  $\times$

steady state: superscript  $*$

thermodynamic equilibrium: superscript  $eq$

subscripts:

spatial subvolumes:  $i, j, \dots = 1, \dots, I$

background:  $B$

ecosystem:  $E$

source:  $S$

particle types:  $p, q, \dots = 1, \dots, P$

biotic species:  $b, b', \dots = 1, \dots, B$

consumer:  $C$

omnivore:  $O$

predator:  $P$

resource:  $R$

waste:  $W$

processes:  $\alpha, \beta, \dots = 1, \dots$

chemical reactions:  $\kappa = 1, \dots, K$

abiotic and biotic conversion:  $AC$  and  $BC$

biomass decay:  $BD$

biomass recycling:  $BR$

biomass synthesis:  $BS$

ecosystem metabolism:  $EM$

resource uptake:  $RU$

growth of species  $b$  on  $b'$ :  $gbb'$

anabolism of species  $b$ :  $ab$

catabolism of species  $b$ :  $cb$

total decay of species  $b$ :  $db$

basal maintenance of species  $b$ :  $mb$

biomass turn-over of species  $b$ :  $tb$

microscopic path:  $\Gamma$

Abiotic parameters: mostly Greek letters.

conversion rates  $\kappa_\alpha$   
 exchange rates  $\alpha_R$  and  $\alpha_W$   
 Biotic parameters: mostly Latin letters.  
 specific growth rate of  $b$  on  $b'$ :  $g_{bb'}$   
 decay rate:  $d_b$   
 recycling ratio:  $r_b$   
 yield:  $q_{bb'}$   
 Variables:  $C$   
 concentrations:  $C_{ip}$   
 temperatures:  $T_i$   
 General quantities  
 affinities:  $A_\alpha$  ( $= TX_\alpha$ )  
 efficiency:  $\eta$   
 entropy production:  $\sigma_\alpha$   
 fluxes:  $F_\alpha$   
 goal function:  $Gf$   
 thermodynamic driving forces:  $X_\alpha$   
 thermodynamic gradient ('linearized' expression of the total external driving force  $X^0$ ):  $\Delta$

## Bijlage C

# Samenvattingen

### C.1 Samenvatting voor het brede publiek

#### **Twee domeinen van wetenschap: thermodynamische fysica en ecosysteem-ecologie**

Zoals de titel 'Energie en Ecologie' suggereert, is dit werk een voorbeeld van wetenschappelijk onderzoek waarbij twee verschillende disciplines met elkaar in contact komen. Het is als het ware het bouwen van een brug waardoor twee velden in het uitgebreide landschap van de wetenschap met elkaar worden verbonden. Het eerste veld is dat van de fysica, die de fundamentele wetten en krachten van het heelal bestudeert, de onderlinge interacties tussen de basiselementen energie, materie, ruimte en tijd. Het tweede is de ecologie die voornamelijk interacties tussen biologische organismen onderling evenals de relaties met hun niet-levende omgeving bestudeert.

Wetenschappers die werken op deze twee velden spreken vaak een iets andere taal. Zoals we zullen zien, zijn het vooral twee domeinen binnen deze twee velden die we trachten te verzoenen. De *thermodynamica* is het domein binnen de fysica dat zich bezighoudt met een 'macroscopische' beschrijving van energieprocessen. Belangrijke begrippen zijn 'efficiëntie', 'temperatuur', 'warmte' en 'arbeid'. Deze thermodynamica heeft toepassingen in vloeistof- en klimaat-systemen. Denk maar aan het warmtetransport in de atmosfeer.

Daartegenover staat de *ecosysteem-ecologie*, het domein binnen de ecologie dat zich bezighoudt met structuren en functionele processen op een schaal groter dan individuele organismen, populaties of leefgemeenschappen. Hierbij spelen begrippen zoals 'biomassa', 'productie', 'biodiversiteit', 'stabiliteit' en de 'voedselketen' een belangrijke rol. Een integratie van beide domeinen, een thermodynamica van ecosystemen, zal hopelijk leiden tot talrijke nieuwe inzichten en toepassingen. Het zal blijken dat deze recente onderzoekstak, de thermodynamische ecologie, merkwaardige verbanden heeft met de thermodynamica van vloeistof- en klimaatsystemen.

#### **Twee theorieën: Darwin vs. Clausius, orde of wanorde?**

In 1859 schreef Darwin zijn beroemde boek "Over de oorsprong van verschillende soorten door middel van natuurlijke selectie, of het behoud van begunstigde rassen in de strijd om het bestaan". Op deze manier konden de ecologen

de 'geordende complexiteit' die we in de levende natuur zien, beter begrijpen. Door willekeurige genetische mutaties gevolgd door een selectieproces waarbij de slechte mutanten uitsterven, is er een evolutie over miljarden jaren, van eenvoudige cellen naar heel complexe (maar toch 'ordelijke') organismen. De aarde vertoont vaak een groei in 'orde'.

Maar in diezelfde 19de eeuw werd ook de thermodynamica verder uitgewerkt. Slechts enkele jaren na Darwin schreef de fysicus Clausius: "... de entropie van het universum streeft naar een maximum." Naast de energie is ook de *entropie* zeer fundamenteel in de thermodynamica. Ze is één van de subtielste en moeilijkste concepten in de fysica. Entropie is een maat voor 'wanorde'. Neem een glas water met een klontje suiker. In tegenstelling tot de gekristalliseerde suikermoleculen, bewegen de moleculen van het water veel meer en veel chaotischer. Breek nu het klontje suiker in kleinere stukjes. Dan stijgt de wanorde in het glas. Wordt het klontje meer en meer stukgebroken, dan eindigen we met een homogene suikeroplossing. De microscopische beweging van de water- en suikermoleculen is nu heel wanordelijk. De entropie is gestegen. Dit gebeurt in de natuur spontaan en is onomkeerbaar; dat is de reden waarom het klontje smelt. Het is onomkeerbaar, want men ziet niet het omgekeerde proces waarbij alle opgeloste suikermoleculen vanzelf terug een heel suikerklontje gaan vormen. Valt het glas op de grond, dan breekt het in duizend stukjes, en wordt er nog meer entropie geproduceerd. Ook hier wordt het omgekeerde proces niet waargenomen. Ruimen we de glasscherven op en lijmen we ze terug aan elkaar, dan verhoogt bijvoorbeeld onze ademhaling, en dan zal daardoor de wanordelijke beweging van de luchtmoleculen weer toenemen. Alle onomkeerbare, spontane processen produceren dus entropie, wanorde. Alles is in 'verval'. Het bovenstaande citaat van Clausius is een formulering van de (bepaalde of beruchte) tweede hoofdwet van de thermodynamica.

We komen dus tot een schijnbare contradictie: de fysica zegt dat de wanorde toeneemt, de ecologie zegt dat ecosystemen kunnen evolueren naar meer orde door de geordende complexiteit van organismen. Hoe valt dit te rijmen indien ecosystemen ook fysische systemen zijn die zouden moeten voldoen aan de wetten van de thermodynamica? Neem opnieuw een glas, en vul het met rivierwater, vol bacteriën en andere organismen. Dit is ons ecosysteem, met veel orde. Als de levende organismen sterven, stijgt de entropie. Om dat te voorkomen voegen we voedsel toe, bv. een schepje suiker, dat de bacteriën kunnen opeten om te groeien. Die suikermoleculen zijn echter ook zeer geordend, want die suikers komen bijvoorbeeld van planten. En die hebben weer 'ordelijke' energie gekregen van de zon. De 'energetische orde' van de suikers wordt omgezet in de geordende complexiteit van de organismen. Maar bij dit proces wordt ook een deel van de suikers verbrand (chemisch geoxideerd) tot  $CO_2$  met veel entropie, en die  $CO_2$ -entropie verdampst uit het glas.

Samengevat: ook al hebben de bacteriën zelf weinig entropie, toch *produceren ze veel entropie* doordat het voedsel wordt afgebroken of gedegradeerd. We zeggen dat het ecosysteem 'ver' uit thermodynamisch evenwicht wordt gedreven' door de toevoer van voedsel. Thermodynamisch evenwicht is de toestand met maximale entropie (voor een gegeven energie), maar door het voedsel heeft het ecosysteem veel minder entropie dan wat maximaal mogelijk is. Het voedsel heeft energie met hoge energetische kwaliteit, dus weinig entropie, en het afvalproduct  $CO_2$  heeft een lage energetische kwaliteit. Dat kwaliteitsverschil waaraan het ecosysteem onderworpen is, noemen we de *'thermodynamische drij-*

*vende kracht*'.

### **Twee uitdagingen: het vreemde gedrag van wervelingen en organismen**

Niet alleen ecosystemen vertonen orde, ook zuiver fysische systemen die ver uit thermodynamisch evenwicht zijn, kunnen geordend zijn. Denk maar aan de soms regelmatige patronen in wolkenformaties of de rimpels in het strand. Een van de grote uitdagingen binnen de fysica is het begrijpen van dergelijke systemen ver uit thermodynamisch evenwicht. Vooral vloeistoffen zijn hierbij interessant. Een bekend experiment is het zogenaamde convectiesysteem bestudeerd door Bénard in 1901. Beschouw een horizontale gas- of vloeistoflaag (bv. olie in een pan), waarbij de onderkant wordt opgewarmd. Het temperatuurverschil tussen onder- en bovenkant is een belangrijke grootte, die dienst doet als een thermodynamische drijvende kracht. Wanneer het temperatuurverschil nul is en de vloeistof niet stroomt, dan is ze in thermodynamisch evenwicht. Bij kleine temperatuurverschillen zal er warmtegeleiding plaatsvinden van de onderkant naar de bovenkant van de vloeistoflaag. Deze warmtegeleiding produceert entropie.

Maar warmen we de onderkant nog sterker op, dan kan er zich een merkwaardig fenomeen voordoen: van zodra het temperatuurverschil een *kritische drempelwaarde* heeft overschreden, begint de vloeistof rond te draaien en te stromen. De vloeistof beweegt bv. eerst naar links, gaat dan omhoog, vervolgens naar rechts en daalt uiteindelijk terug om opnieuw aan deze cyclus te beginnen. Deze werveling vormt wat men noemt een '*convectiecel*', en talrijke convectiecellen samen organiseren zich tot bv. een horizontaal uitgestrekt zeshoekig honingraatpatroon. In het midden van de zeshoekjes beweegt de vloeistof omhoog, aan de randen daalt ze.

Wat vooral belangrijk is, is dat door deze stromende convectiecellen het warmtetransport en de entropieproductie groter worden. Hetzelfde fenomeen doet zich voor in de atmosfeer: talrijke wervelingen, windstromen, orkanen,... ontstaan omdat de grond of het zeewater door de zon wordt opgewarmd. Ook oceaanstromen kunnen zo worden beschreven. En ook het globale klimaatstelsel wordt gedreven door een warmtetransport van de tropen naar de polen, omdat de tropen door de zon sterker worden opgewarmd dan de polen. Dit verschil in opwarming geeft een drijvende kracht, waardoor oceaen- en luchtstromen (inclusief wolken,...) ontstaan. Waarom gedraagt de vloeistof of de lucht zich zo vreemd? Hoe kunnen we het ontstaan van wervelingen beter begrijpen? Hoe snel bewegen ze? Kortom: *waardoor worden deze toestanden gekarakteriseerd?*

Ook de ecologie heeft een grote uitdaging, het begrijpen van ecologische mechanismen. Die uitdaging is eigenlijk zeer analoog aan het bovenstaande. Waarom gedraagt een ecosysteem, dat door een doorstroom van energie uit thermodynamisch evenwicht wordt gedreven, zich zo vreemd? Hoe kunnen we het ontstaan van levende organismen beter begrijpen? Hoe snel groeien ze? Kortom: *waardoor wordt leven gekarakteriseerd?*

### **Een gemeenschappelijke strategie: maximum of minimum?**

Om bovenstaande vragen te beantwoorden, maken zowel fysici, onder wie sommige klimatologen, alsook sommige ecologen gebruik van een bepaalde strategie. Ze zoeken naar (wiskundige) '*extremumprincipes*'. Dat zijn principes

waarbij een bepaalde grootheid maximaal of minimaal wordt. Daardoor kunnen ze het gedrag van complexe (maar vaak ordelijke) systemen beschrijven en verklaren. Het gebruik van extremumprincipes geeft een eerste aanzet tot een speciale overeenstemming tussen de twee wetenschappelijke velden.

Laten we eerst kijken naar de fysica. Als meest eenvoudige voorbeeld kunnen we een balletje in een kom beschouwen. Waar komt het balletje uiteindelijk tot rust? Het blijkt dat men dergelijke vraag kan beantwoorden door te kijken naar een eenvoudige wiskundige grootheid, namelijk de hoogte in de kom. Waar de hoogte minimaal is, het laagste punt in de kom, daar komt het balletje tot rust. Eigenlijk houdt dit voorbeeld op een subtiele manier reeds verband met de hierboven vernoemde tweede hoofdwet, die zegt dat de entropie (van het heelal of een geïsoleerd systeem) streeft naar een maximum, wat opnieuw een extremum is.

Maar er zijn nog meer voorbeelden te vinden: neem opnieuw de opgewarmde vloeistoflaag, waarbij het uitwendige temperatuursverschil klein en constant is. Dan zal de entropieproductie (afgekort tot 'EP') volgens Prigogine (1947) streven naar een minimum. Brengen we een kleine verstoring aan in de vloeistoflaag, door bv. eventjes te roeren, dan zal de EP eventjes groter worden, om vervolgens terug spontaan te dalen naar de minimale waarde.

In de wereld van de ecologie wordt ook gezocht naar een universeel principe om het gedrag van ecosystemen te begrijpen. Voor een complex ecosysteem is het heel moeilijk om te bepalen of het 'optimaal' functioneert. Wanneer is een ecosysteem bijvoorbeeld door de mens 'verstoord'? Sommige ecologen zouden willen kunnen spreken over 'zieke' en 'gezonde' ecosystemen. Ze nemen daarbij als analogie het menselijk lichaam. Dat functioneert optimaal bij een temperatuur (opnieuw een belangrijke thermodynamische grootheid) van ongeveer 37°C. Is het lichaam ziek, dan kan de temperatuur afwijken van de optimale waarde. Net zoals ons lichaam, zijn ook ecosystemen voorbeelden van complexe, zelforganiserende, zelfregulerende systemen. Daar de menselijke activiteit de werking van ecosystemen kan verstoren, wat vaak resulteert in ernstige gevolgen, zijn ecologen op zoek naar wat ze noemen *ecologische doelfuncties* om de ernst van die verstoringen in te schatten.

Dergelijke doelfuncties zijn in wezen niets anders dan de grootheden in extremumprincipes. Het geloof in het bestaan van ecologische doelfuncties ligt voornamelijk in de zogenaamde climaxtheorie: een platgebrand of gekapt bos kan (maar dat is niet altijd zo) via een opeenvolging van stadia (pioniersplantjes, kleine struiken, grote bomen) opnieuw evolueren naar een relatief stabiele en optimaal functionerende eindtoestand, de climax, een volgroeid bos. De eerste voorstellen van doelfuncties voor dergelijke climaxsystemen waren voornamelijk ecologische grootheden, zoals biomassa die maximaal zou worden in de climaxtoestand. Maar door de successen van de thermodynamische grootheden (entropie, entropieproductie, temperatuur) in talrijke systemen, zijn sommige ecologen gaan zoeken naar thermodynamische doelfuncties, met soms vreemde namen zoals eco-exergie, ascendentie of emergie.

De tweede hoofdwet legt thermodynamische voorwaarden op aan de evolutie van (eco)systemen. Niet zomaar alles kan spontaan verlopen. De vraag is of men ook door bijvoorbeeld een goed begrip van thermodynamische ecologische doelfuncties voorwaarden en beperkingen op de evolutie en de structuur van ecosystemen kan afleiden. Sommigen hopen dat men zo bijvoorbeeld de biodiversiteit, de lengte van een voedselketen de mate van competitie of de efficiëntie

van energie-omzettingsprocessen bij organismen kan verklaren met behulp van de thermodynamica.

Voorlopig is er echter nog geen algemeen door natuurkundigen aanvaard extremumprincipe voor systemen ver uit thermodynamisch evenwicht. Ook binnen de ecologische wetenschap is er nog volop discussie over het idee van doelfuncties. Vaak zijn ze moeilijk te bepalen en zijn ze nauwelijks experimenteel te meten en te testen.

### Maximum en minimum entropieproductie

Hoewel er (nog) geen algemeen aanvaard extremumprincipe bestaat, zijn er toch een aantal argumenten te geven om entropieproductie te bestuderen.

- 1) De EP is de toename van de entropie in de tijd. Ze combineert dus een basisgrootheid van de thermodynamica, de entropie, met een basisbegrip van de dynamica, de tijd. Dit vertaalt zich in een mooie wiskundige uitdrukking voor de EP. Die is te schrijven als het product van de oorzaak, de drijvende kracht, met het gevolg, de resulterende stroom. Vergelijk het met een rivier, waarbij de kracht, de helling, vermenigvuldigd wordt met de stroomsnelheid.
- 2) We hebben gezien dat de tweede hoofdwet zegt dat er altijd wanorde wordt geproduceerd bij elk spontaan, irreversibel proces. Des te irreversibeler, des te meer EP. De tweede hoofdwet zegt echter nog niet hoe groot de EP dan wel moet zijn.
- 3) We hebben ook vermeld dat Prigogine aantoonde dat de EP voor een systeem onderworpen aan een heel kleine drijvende kracht streeft naar een minimum (het MinEP-principe). Voor dergelijke systemen dicht bij evenwicht is EP dus een doelfunctie.

Maar het is vooral het werk van enkele klimatologen dat de EP meer in de belangstelling bracht bij een aantal wetenschappers. In 1979 berekende Paltridge het gemiddelde warmtetransport (als gevolg van alle oceaan- en atmosfeerstromen) van de tropen naar de polen. Hij kwam daarbij tot een merkwaardige vaststelling: de warmtestroom ligt relatief dicht bij een speciale waarde, waarbij de totale EP van alle warmtetransportprocessen op aarde maximaal zou zijn. Zoals we weten is deze EP te schrijven als de drijvende kracht (ruwweg het gemiddelde temperatuurverschil tussen tropen en polen) maal de warmtestroom. Beschouw opnieuw een rivier. De hypothese luidt dat een rivier alle mogelijke trajecten en processen, zoals het ontstaan van draaikolkjes, zou opzoeken opdat de EP maximaal zou worden.

Later werd deze '*maximum entropieproductie*' (MaxEP) hypothese verfijnd en toegepast op talrijke andere systemen. Vaak ging dat gepaard met enige verwarring: Prigogine zegt "minimum EP", en Paltridge zegt "maximum EP". Hoe kan dat? Maar zelfs binnen de MaxEP-literatuur was er veel onduidelijk. Een 'maximum' wil zeggen 'hoger dan de rest', maar wat bedoelt men eigenlijk met 'de rest'? Wat zijn de aannames? Wat zijn de andere toestanden? Welke EP van welk proces wordt precies gemaximaliseerd? En wat is de (experimentele) status: is het een voorlopige hypothese of is het reeds een sterker principe met een stevig bewijs? Kortom, veel is onduidelijk. Een groot deel van mijn onderzoek bestond er dan ook in de ganse literatuur te doorpluizen en allerlei knopen te ontwarren. De conclusie is dat er naast Prigogines MinEP niet minder dan 9 verschillende MaxEP-hypotheses (en principes) bestaan. En daarnaast zijn er nog een paar andere gerelateerde EP-hypotheses. Het is mogelijk om ze allemaal netjes schematisch te klasseren, maar daar gaan we hier niet verder op in.

De kritische studie van de literatuur bracht ook aan het licht dat enkele voorgestelde wiskundige bewijzen voor MaxEP nog verre van voldoende blijken te zijn.

### Entropieproductie in ecosystemen

Het MaxEP-idee van Paltridge is wel intrigerend. Zou er iets analoogs kunnen bestaan voor ecosystemen? Wat de wiskundige beschrijving van de MaxEP-hypothese betreft, is er wel degelijk een overeenstemming. Neem opnieuw het glas met water en bacteriën. Laat er continu voedsel instromen. Deze instroom is analoog met de instroom van zonne-energie in de tropen. In het glas-ecosysteem wordt de kwaliteit van dat voedsel door allerlei processen (chemische oxidatie, biologische groei, ademhaling,...) gereduceerd. Dit omzetten en afbreken van voedsel tot afvalproducten (bv.  $CO_2$ ) noemt men het *ecosysteemetabolisme*, en het is gelijkaardig aan het warmtetransport van de tropen naar de polen. Uiteindelijk wordt de  $CO_2$  uit het glas gestoten, net zoals de polen warmtestraling uitzenden naar de ruimte.

Er zijn dus drie belangrijke basisprocessen: de instroom van voedsel, de afbraak van voedsel (het metabolisme) en de uitstroom van afval. Een belangrijk deel van ons onderzoek was het afleiden van een betrouwbare uitdrukking voor de EP van elk van die drie ecosysteemprocessen. Vooral het bepalen van de drijvende krachten was niet eenvoudig, want daarbij raken we aan een kernprobleem in de thermodynamische ecologie: wat is de entropie van een organisme? Die is laag, maar hoe laag? Door een belangrijke beperking, dat het ecosysteem in een stationaire toestand moet zitten, zijn we erin geslaagd dit probleem te ontwijken. Een *stationaire toestand* is een speciale toestand waarbij bijvoorbeeld het aantal of de concentratie aan organismen niet verandert in de tijd. Daardoor zou ook de entropie van de organismen niet veranderen, en die eigenschap maakt het ons veel gemakkelijker. We hebben dus correcte uitdrukkingen gevonden voor de drijvende krachten van de drie basisprocessen, onder de voorwaarde dat het ecosysteem zich in een stationaire toestand bevindt. Ruwweg gesteld worden deze krachten bepaald door concentratieverschillen: als de concentratie van bv.  $CO_2$  in het glas groter is dan die in de lucht, dan zal er een uitstoot van  $CO_2$  zijn. En met nieuwe inzichten omtrent de problematiek van de drijvende krachten, konden we ook kritiek geven op andere uitdrukkingen voor de EP die we aantreffen in de literatuur, maar dat is hier minder relevant.

De vraag is nu of de snelheid van de afbraak van voedsel, het ecosysteemetabolisme, in de buurt ligt van die waarde waarvoor de EP van het ecosysteemetabolisme maximaal is. In een studie met Filip Meysman wordt een aanzet gegeven om deze ecosysteem-MaxEP-hypothese te testen met observaties van sediment ecosystemen op de bodem van de oceaan. Dood organisch materiaal (dode walvissen,...) valt neer op de bodem en dient daar als voedsel voor talrijke organismen. De conclusies blijven voorlopig echter open, want enkele eigenschappen van de chemische oxidatie van dat dood organisch materiaal zijn nog niet voldoende gekend. Ook een verklaring voor MaxEP is er nog niet helemaal, maar er is een mooi voorstel. Het blijkt dat bij heel trage voedselafbraak de corresponderende kracht die het metabolisme drijft, groot is. Deze zogenaamde 'interne' drijvende kracht meet eigenlijk hoe ver het ecosysteem intern uit evenwicht is. Daar het ecosysteem naar evenwicht streeft, is de interne drijvende kracht een soort van interne 'frustratie' die moet worden opgeheven. Dat kan door de voedselafbraak te vergroten. Maar een te groot metabolisme kan wel eens te vermoeiend zijn voor het ecosysteem. Het ecosysteem staat dus

voor een keuze, en ergens tussen de twee uitersten in is er een optimale waarde die het systeem verkiest. Als een dergelijk mechanisme blijkt te bestaan, dan kan men hopen dat die optimale waarde equivalent is aan de MaxEP-waarde.

Met de bekomen uitdrukkingen voor de totale EP (de som van de EP's van de drie processen) kunnen we ook trachten een viertal andere vragen te beantwoorden.

1) Een belangrijk probleem in de ecologie is het bestaan van verschillende stationaire toestanden en de drastische verschuivingen die mogelijk zijn tussen dergelijke toestanden. Kijken we naar een ecosysteem op de oceaanbodem, dan zien we talrijke soorten die met elkaar interageren en samen een stabiele toestand vormen. Een kleine verstoring, bv. een kleine omwoeling, en de verschillende soorten reageren zodat het systeem terug naar de oude toestand evolueert. Maar het is mogelijk dat bij een sterkere verstoring plotseling een drastische verschuiving optreedt in het ecosysteem. Soorten verdwijnen, andere krijgen andere functies, en het systeem evolueert naar een heel andere stationaire toestand. Door bv. menselijke activiteiten zijn dergelijke catastrofale verschuivingen mogelijk in talrijke ecosystemen, denk maar aan woestijnvorming. Ecologen zijn bezorgd omwille van de daling in de soortenrijkdom. Daarom willen ze beter kunnen voorspellen welke stationaire toestand wordt geselecteerd in welke omstandigheden. Dit brengt ons bij de volgende hypothese: is de meest stabiele stationaire toestand ook degene met de hoogste EP? Dit is eigenlijk één van die 9 bovenvermelde MaxEP-hypotheses, niet te verwarren met het idee van Paltridge. Sommige ecologen verwachten een positief antwoord omdat de meest stabiele systemen de meeste processen (met de bijhorende EP) zouden hebben om die stabiliteit te garanderen.

2) Ten tweede kunnen we onderzoeken wat er gebeurt indien het ecosysteem verder uit evenwicht wordt gedreven. Stijgt de EP indien er meer voedsel in het ecosysteem stroomt? Ook deze vraag kan relevant zijn, denk maar aan de positieve en negatieve effecten van (over)bemesting. Hoe past het ecosysteem zich aan? Meer voedsel zou immers meer activiteit kunnen betekenen, meer processen, en bijgevolg meer EP. Net zoals een steilere rivier sneller stroomt.

3) Stijgt de EP onder evolutie? Als er nieuwe soorten verschijnen, die beter aangepast zijn zodat ze meer voedsel opnemen en verwerken, dan kan men verwachten dat de EP groter wordt.

4) Is de EP van een levend ecosysteem groter dan die van een dood ecosysteem? Als een biocide al het leven doodt, terwijl er toch eenzelfde hoeveelheid voedsel instroomt, gaat dan de EP dalen? Heeft een bos een grotere EP dan een dode woestijn? Dit kunnen interessante vragen zijn met betrekking tot de meer filosofische zoektocht naar de 'essentie' van het leven of van systemen ver uit evenwicht. Als de antwoorden op die vragen "ja" zijn, dan wil dat zeggen dat leven meer wanorde produceert. Biologische processen zouden dan spontaner of onomkeerbaarder zijn dan niet-biologische processen. Denken we terug aan de vloeistoflaag die wordt opgewarmd. Bij een kleine opwarming is er warmtegeleiding, maar bij een voldoende grote opwarming ontstaat er convector. Door het stromen van de vloeistof stijgt het warmtetransport en bijgevolg de EP.

Door het bestuderen van verschillende wiskundige modellen voor ecosystemen, kunnen we bovenstaande vragen onderzoeken. Het blijkt dat vooral één bepaald model hiervoor interessant is: een ecosysteem met één soort van *basisconsumenten* en één soort van *omnivoren*. De basisconsumenten zijn organismen die leven van het basisvoedsel, bv. de glucose. Daarnaast zijn er

de omnivoren, die ook rechtstreeks eten van het basisvoedsel, maar ze hebben ook die basisconsumenten zelf als prooi. Doordat ze de basisconsumenten als voedsel hebben, staan ze hoger in de voedselketen. Berekenen we de EP voor dergelijk ecosysteem, dan blijkt jammer genoeg dat we al de vier bovenstaande vragen met "nee" moeten beantwoorden. Voorlopig moeten we dus nog erg wantrouwig staan tegenover het idee van EP als een ecologische doelfunctie, als een maat voor ecosysteemstabiliteit of als een karakterisering voor leven. Ook wat betreft de andere kandidaten voor ecologische doelfuncties (biomassa, totale energiedoorstroom, exergie, emergie, primaire productie,...) moeten we voorlopig kritisch blijven.

Maar misschien is ons omnivoor ecosysteem iets te eenvoudig en niet realistisch genoeg. Vooral wat betreft het laatste, vierde probleem is er nog meer studie noodzakelijk. Bij dit vierde probleem verwezen we opnieuw naar het convectieve vloeistofsysteem, en dit opent een verrassende nieuwe kijk op de werking van zowel ecosystemen als vloeistofsystemen.

### **Twee systemen: de analogie tussen een vloeistofsysteem en een ecosysteem**

Het Bénard-vloeistofsysteem met een constante instroom van warmte-energie en het glas water ecosysteem met een constante instroom van suikers vertonen merkwaardige en dieperliggende gelijkenissen.

Het eerste wat opvalt is dat het uitwendige temperatuurverschil van de vloeistoflaag alsook het energetische kwaliteitsverschil tussen het ingepompte voedsel en de uitstromende  $CO_2$  verband houden met de uitwendige drijvende kracht. Beide systemen vertonen een kritische drempelwaarde voor deze uitwendige kracht. Indien die kracht kleiner is dan deze kritische drempelwaarde, dan zijn de stationaire toestanden gegeven door respectievelijk warmtegeleiding en chemische oxidatie van voedsel. Maar indien de systemen verder uit evenwicht worden gedreven, tot boven de kritische drempelwaarde, dan treden er nieuwe processen op: vloeistofconvectie en biologische activiteit.

We kunnen dus stellen dat de instroom van warmte-energie met een hoge temperatuur in de vloeistof analoog is met de instroom van voedsel in het ecosysteem. En zowel de convectiecellen als de biologische cellen vertonen veel orde. Immers, als de vloeistof gaat rondstromen en regelmatige convectiepatronen gaat vormen, dan is de microscopische beweging van de vloeistofmoleculen minder wanordelijk. En de beweging van de moleculen in biologische organismen mag ook niet wanordelijk verlopen.

Deze analogie is niet louter een kwestie van beschrijving. Omdat het Bénard-vloeistofsysteem zeer relevant is in de klimaatwetenschappen - het gedraagt zich immers net zoals grote atmosferische luchtstromen - was het de klimatoloog Lorenz die in 1963 een drietal wiskundige vergelijkingen afleidde voor dit vloeistofsysteem. Deze vergelijkingen werden beroemd omdat ze door de opkomst van de computer een nieuwe impuls gaven aan een populair geworden onderzoekstak in de wiskunde: de chaostheorie. Drie grootheden zijn cruciaal: de gemiddelde snelheid van de vloeistofstroming, de temperatuur in de onderkant van de vloeistoflaag, en het temperatuursverschil tussen de opgaande en de neergaande vloeistofstromingen. De drie vergelijkingen beschrijven hoe deze drie grootheden variëren in de tijd. Ze zijn voldoende om bijvoorbeeld het bestaan van bovenvermelde kritische drempelwaarde wiskundig aan te tonen.

Daarnaast kunnen we het meest eenvoudige ecosysteem bestuderen, dat be-

staat uit twee fundamentele grootheden: de hoeveelheid voedsel in het glas, en de concentratie van de bacteriën. Opnieuw kunnen we bestuderen hoe die veranderen in de loop van de tijd, met behulp van twee vergelijkingen.

Is er een verband tussen die wiskundige vergelijkingen? Dat blijkt inderdaad zo te zijn, en we mogen gerust deze vondst als het meest waardevolle aspect van het onderzoek beschouwen. Door een kleine aanname kunnen we de drie vergelijkingen van Lorenz herschrijven tot twee vergelijkingen, en die kunnen dan weer herschreven worden totdat ze wiskundig van exact dezelfde vorm zijn als de ecosysteemvergelijkingen! Zo kunnen we de volgende overeenkomsten aantonen:

\*De temperatuur (of de warmte-energie) in de onderkant van de vloeistoflaag komt overeen met de voedselconcentratie, de gemiddelde temperatuur in het midden of aan de bovenkant komt overeen met de concentratie aan afvalproducten. Het temperatuursverschil in de vloeistoflaag is dus analoog aan het concentratieverschil in het waterecosysteem.

\*De bewegingsenergie van de ronddraaiende convectiecellen komt overeen met de concentratie aan basisconsumenten in het ecosysteem.

\*Het vloeistofsysteem had een kritische drempelwaarde voor het uitwendige temperatuurverschil. Als deze uitwendige drijvende kracht te laag is, dan kunnen de convectiecellen niet overleven, en hun bewegingsenergie streeft naar nul. Ook bij ecosystemen is er een kritische drempelwaarde: stroomt er te weinig voedsel in het ecosysteem, dan kunnen de bacteriën daar niet van overleven, en streeft de concentratie naar nul. Alles sterft dus uit. De stationaire toestand is dood. Maar van zodra er voldoende eten beschikbaar is, kunnen de organismen wel overleven en het ecosysteem evolueert naar een stabiele stationaire waarde voor de concentratie aan basisconsumenten. Dat is net zoals het vloeistofsysteem evolueert naar een stabiele stationaire waarde voor de bewegingsenergie.

\*Warmte-energie met een hoge temperatuur wordt omgezet in bewegingsenergie van de vloeistof. Dit komt door de Archimedeskracht: warme vloeistof heeft een lagere dichtheid dan koude vloeistof. Warmen we de onderkant van de vloeistoflaag op, dan daalt daar de dichtheid. De bovenkant van de laag wordt dus relatief zwaarder. Als die voldoende zwaar is, wil die naar beneden zakken, en zo wordt de verticale vloeistofstroming in gang gezet. Dit proces is te vergelijken met biologische groei, waarbij voedsel wordt omgezet in biomassa.

\*Door interne wrijving wordt de snelheid afgeremd, want anders zou die oneindig groot worden. Hierdoor wordt de bewegingsenergie omgezet in warmte-energie met een lage temperatuur. Dat is net zoals biologische cellen die afsterven, want als er geen sterfte was, dan zou de concentratie aan organismen oneindig groot worden. Door deze celdood wordt biomassa afgebroken.

\*Het totale warmtetransport in het vloeistofsysteem is te vertalen naar het ecosysteemmetabolisme.

\*Het warmtetransport stijgt als de convectiecellen beginnen rond te draaien. Ook voor ons meest eenvoudige ecosysteem stijgt de totale voedselafbraak onder biologische activiteit. Als we terugdenken aan de vierde vraagstelling in vorige sectie, dan zien we dat voor dit specifieke ecosysteem de EP in de levende stationaire toestand wel groter is dan in de dode toestand.

\*Het volledige Lorenzmodel bestaat uit drie vergelijkingen en drie grootheden i.p.v. twee. Kunnen we een ecosysteemanalogie opstellen voor de derde grootheid, het temperatuursverschil tussen de stijgende en de dalende vloeistof? Er blijkt inderdaad een mogelijkheid te zijn om het Lorenzmodel te vertalen naar

een model dat een benadering geeft voor biologische celgroei. De derde grootte zou dan de rol kunnen spelen van de concentratie van een extra chemische stof, zoals een enzyme, die nodig is bij celgroei.

### **Twee toepassingen: competitie en predatie**

Bovenstaande wiskundige analogie heeft mooie toepassingen waarvan we er hier twee bespreken. Twee belangrijke ecologische interacties, competitie en predatie, zullen worden vertaald naar het vloeistofsysteem.

In de ecologie is er het bekende fenomeen van 'competitieve exclusie'. Stel we laten verschillende soorten basisconsumenten vrij in ons eenvoudig glas-water-ecosysteem. Men heeft aangetoond dat indien er slechts één soort voedselbron (suiker) is, de soort met de hoogste 'biologische fitness' (overlevingswaarde) kan overleven en de minder sterke soort zal uitsterven. Deze fitness wordt wiskundig weergegeven door de verhouding van de groeisnelheid en de sterftegraad. Des te sneller de groei of des te lager de sterfte, des te sterker het organisme.

Welnu, met behulp van de wiskundige equivalentie kunnen we de fitness vertalen naar het vloeistofsysteem. De consumenten worden nu convectiecellen, en het voedsel wordt warmte-energie. Zoals we reeds weten, kunnen er boven de kritische drempelwaarden spontaan convectiecellen ontstaan. De vraag is: welk convectiepatroon wordt er uiteindelijk geselecteerd en hoe groot zijn deze convectiecellen? Zijn ze breed of smal? Als ze te smal zijn, dan is de 'sterftegraad' van de convectiecel door de interne wrijving te hoog. Maar zijn ze te breed, dan werkt de Archimedeskracht minder goed, en dan ligt de 'groeisnelheid' te laag. Het blijkt dus dat de 'vloeistoffitness' afhankelijk is van de grootte van de convectiecellen. Verschillende soorten cellen treden met elkaar in competitie en degene met de hoogste vloeistoffitness zal overwinnen en zal het uiteindelijke patroon bepalen. Op deze manier kunnen we berekenen wat de best aangepaste grootte van een convectiecel is. Onze berekende waarde blijkt precies overeen te stemmen met wat men vroeger door experimenten heeft bepaald. Lord Rayleigh was ons echter voor, want hij had reeds in 1916 een correcte wiskundige verklaring voor de geobserveerde grootte van de cellen gevonden. Maar het is toch merkwaardig dat we nu een andere wiskundige afleiding kunnen geven, die gebaseerd is op ecologische principes. Het bevestigt en versterkt de correspondentie tussen de twee soorten systemen.

Een tweede interessante toepassing heeft te maken met predatie. Laten we eens kijken wat er gebeurt als we een predator in ons glas-water-ecosysteem brengen. Deze predator eet de basisconsumenten, maar als die hun concentratie te laag is, dan kan de predator niet overleven. Maar stijgt de drijvende kracht, dan stijgt de concentratie aan basisconsumenten. Er blijkt een tweede kritische drempelwaarde te bestaan. Als de drijvende kracht hierboven komt, dan kunnen de predatoren wel overleven. De vraag is: hebben deze predatoren een analogon in het vloeistofsysteem? Onze hypothese luidt dat de concentratie aan predatoren overeenkomt met nieuwe bijdragen in de bewegingsenergie. Als het temperatuurverschil over de vloeistoflaag groter wordt, kan het een tweede kritische drempelwaarde passeren. Voorbij deze drempelwaarde wordt het oude convectiepatroon onstabiel en ontstaat er een nieuw patroon, met bv. extra draaiing in de cellen. Dit geeft nieuwe bijdragen in de bewegingsenergie van de vloeistof.

Hoewel we nog niet in staat zijn om wiskundig aan te tonen dat het predatie-ecosysteem equivalent is met het vloeistofsysteem voorbij de tweede drempel-

waarde, kunnen we wel kijken naar enkele voorspellingen van onze hypothese. Het blijkt dat de introductie van predatoren het totale ecosysteemmetabolisme doet dalen. Dat geeft dus ook een daling in EP. Zou het systeem een verhoging van EP verkiezen, dan was het liever de predatoren kwijt dan rijk. Welnu, verschillende studies van het warmtetransport bij convectieve vloeistofsystemen laten inderdaad zien dat de EP en het warmtetransport van het nieuwe convectiepatroon voorbij de tweede drempelwaarde lager is dan bij het oude convectiepatroon. Dit zou onze hypothese kunnen bevestigen, maar het is nog geen bewijs.

### **Naar een unificatie van de twee soorten systemen**

Met bovenstaande analogie kunnen we tot slot wat verder speculeren en filosoferen over een mogelijke unificatie in de beschrijving van zowel fysische systemen (vloeistofsystemen, klimaatsystemen,...) als ecologische systemen (bossen, oceaانبodems,...).

Het klimaatsysteem kunnen we onderverdelen in vier compartimenten: de zon, de tropen, de polen en de interstellaire ruimte. Zo ook kunnen we het glaswater-ecosysteem onderverdelen in het voedsel buiten het glas, het opgeloste voedsel in het glas, de  $CO_2$  in het glas en de  $CO_2$  in de lucht. De biologische processen in het ecosysteem komen overeen met atmosferische (en eventueel ook oceanische) processen. In de atmosfeer zijn er grote luchtstromen waarop kleinere luchtstromen als het ware predateren. Ze tappen bewegingsenergie af van de grotere stromingen. Of kijken we naar orkanen, dan zien we ook de grote werveling met daarin kleinere wervelingetjes, en daarin nog kleinere wervelingetjes. Dit noemt men de '*Kolmogorov-waterval*'. Eigenlijk ontstaat er zo als het ware een keten van allerlei soorten luchtwervelingen die elkaar 'opeten', net zoals een voedselketen in de ecologie, een zogenaamde '*trophische waterval*'. Bovendien kunnen deze wervelingen in competitie treden, er kunnen 'omnivoor' wervelingen opduiken, de wervelingen kunnen langzaamaan wijzigen (zoals genetische mutaties bij organismen), evolueren, groeien, uitsterven, andere wervelingen aanmaken en zich zo als het ware voortplanten. Vloeistofsystemen, orkanen of het ganse klimaatsysteem kunnen dus beschreven worden met termen uit de ecologie. En ecologische systemen kunnen beschreven worden met termen uit de fysica, zoals de thermodynamica.

Als de atmosfeer bestaat uit talrijke soorten complexe interagerende wervelingen, dan kunnen die samen eventueel een tamelijk eenvoudig 'emergent' gedrag vertonen, zoals bv. het fenomeen massahysterie dat kan optreden bij een volksmassa van talrijke individuen. Sommige wetenschappers hopen dat indien het klimaat of het ecosysteem een dergelijk emergent gedrag vertoont, dit resulteert in een maximalisatie van de EP die hoort bij het atmosferisch warmtetransport of het ecosysteemmetabolisme. Of MaxEP op dergelijke manier blijkt te werken is nog maar de vraag. (Deze MaxEP-hypothese van Paltridge mag niet worden verward met de bovenvermelde effecten van predatoren of omnivoren op het verhogen of verlagen van de EP. Het zijn twee totaal verschillende hypothesen.)

Nog verder speculerend kunnen we ons vragen stellen bij de oorsprong van het leven. Als vloeistofsystemen ver uit evenwicht worden gedreven, dan kunnen kleine spontane fluctuaties als vanzelf uitgroeien tot macroscopische geordende structuren. Een toevallige geordende beweging van moleculen kan uitgroeien tot een convectiecel of een orkaan. Zo ook groeiden een paar miljard jaar geleden

toevallige interacties van chemische stoffen uit tot de eerste levende cellen. Er is wel een verschil in complexiteit, want vloeistofstromen ontstaan gemakkelijker dan levende cellen, en levende processen bestaan uit talrijke complexe interacties tussen talrijke soorten moleculen. Maar het onderliggende basismechanisme of principe kan wel hetzelfde zijn. Zou dit alles een unificatie kunnen betekenen tussen de niet-levende fysische systemen en de levende ecosystemen?

### Conclusie van het onderzoek

We hebben gezien dat een groot deel van het onderzoek uit niets anders bestond dan het geven van kritiek op het werk van anderen. Een kritische ingesteldheid is als wetenschapper erg belangrijk. We willen immers niet zomaar blindelings mooie theorieën aanhangen. Zo hebben we nieuwe kritische inzichten bekomen bij het opstellen van een schematische classificatie van talrijke ideeën m.b.t. de EP van systemen. Ook hebben we een uitdrukking voor de EP in ecosystemen afgeleid, die iets rigoureuzer is dan wat men tot nu toe in de literatuur aantrof. En met deze EP konden we aan de slag om allerlei hypothesen te testen en, zoals bleek, te weerleggen.

Maar we zijn er ook in geslaagd om een positiever, constructiever verhaal te brengen, een uitdagend idee, dat zelfs een gans nieuw onderzoeksproject kan openen. Ecosystemen gedragen zich heel analoog aan convectieve vloeistof- en atmosfeersystemen. Tot nog toe gaf deze brug die we bouwden tussen de wereld van de fysica en de wereld van de ecologie geen nieuwe, niet-triviale resultaten. Vanuit esthetisch oogpunt is het idee wel mooi, en we zijn erin geslaagd om reeds gekende theorieën van de ene wereld te vertalen in reeds gekende aspecten van de andere wereld. Een voorbeeld hiervan was de afleiding van de grootte van een convectiecel met behulp van ecologische competitie. De hoop is dat deze wetenschappelijke 'steen van Rosette' het mogelijk zal maken om ook onbeantwoorde vraagstukken in de ene wereld op te lossen met behulp van technieken uit de andere wereld.

## C.2 Wetenschappelijke resultaten

Laat ons hier de 'sappigste' resultaten van ons onderzoek overlopen. Die kunnen misschien het best samengevat worden met de volgende formulering: *er is een correspondentie op verschillende schalen van complexiteit tussen aan de ene kant fysische systemen, in het bijzonder het warmtetransport in vloeistoffen en gassen, en aan de andere kant ecologische systemen, in het bijzonder het ecosysteemmetabolisme*. Fig. 1.2 toont deze correspondentie, de wetenschappelijke 'steen van Rosette'.

De 'megascopische' schaal is het meest complexe niveau van beschrijving. Op dit niveau is er een analogie tussen bv. het klimaatstelsel met verschillende types van wervelingen (Hadleycellen, orkanen, kleine eddies,...) aan de ene kant en complexe ecosystemen zoals oceaan-sediment-ecosystemen of chemostaten met verschillende soorten organismen (eencelligen, wiertjes, geleedpotigen,...) aan de andere, zie fig. 1.3.

Zowel de aarde als het sedimentecosysteem hebben een instroom van energie met hoge kwaliteit: hoge-frequentie-warmtestraling of organisch en chemisch materiaal met een hoge chemische potentiaal. Deze energie wordt omgezet tot energie van lage kwaliteit die uit het systeem wordt gestoten: lage-frequentie-

straling of geoxideerde afvalproducten zoals  $CO_2$  verlaten de aarde of het sediment. Voor het klimaatsysteem wordt energie getransporteerd door conductie en convectie van warmte van de tropen naar de polen. Het sediment heeft een ecosysteemmetabolisme, waarbij chemische en biologische processen het voedsel verbranden. In fig. 1.3 worden deze belangrijkste processen weergegeven door pijlen met dikke randen.

Fig. 1.4 geeft een meer abstracte beschrijving die laat zien dat beide systemen een functionele gelijkenis hebben. Daar de megascopische beschrijving te complex is, gaan we hier enkel de meest basale werking beschrijven. Het model universum wordt onderverdeeld in de omgeving en het systeem, en beide hebben twee compartimenten, één voor het voedsel, de energetische hulpbron, en één voor het afval. Door te kijken naar de energie en massabalansen kunnen we de dynamica van de twee systeemvariabelen opschrijven als het verschil tussen de instroom en de uitstroom van de respectievelijke compartimenten.

$$\frac{dC_R}{dt} = \alpha_R(C_R^0 - C_R) - \kappa^\times(C_R - C_W/K_{eq}), \quad (C.1)$$

$$\frac{dC_W}{dt} = \kappa^\times(C_R - C_W/K_{eq}) - \alpha_W(C_W - C_W^0). \quad (C.2)$$

Voor het ecosysteem zijn  $C_R$  en  $C_W$  het voedsel en de  $CO_2$ . De superscript 0 verwijst naar de constante omgevingsgrootheden,  $\alpha_R$  en  $\alpha_W$  zijn specifieke uitwisselingssnelheden door diffusie of actief transport, en  $\kappa^\times$  is de specifieke afbraaksnelheid van het voedsel. Het superscript  $\times$  verwijst naar het feit dat dit een 'effectieve' snelheid is: in het algemeen is  $\kappa$  afhankelijk van de verschillende extra (verborgen) variabelen in het systeem, zoals de concentraties van de organismen. Maar we veronderstellen dat het voedselweb in een quasistationaire toestand zit, zodat  $\kappa^\times$  enkel afhangt van de twee overblijvende variabelen  $C_R$  en  $C_W$ .  $K_{eq}$  is de evenwichtsconstante voor de chemische oxidatiereactie van voedsel (bv. suiker) naar afval.

Ons eerste resultaat is dat deze quasistationaire dynamica vertaald kan worden naar een sterk vereenvoudigd klimaatsysteem in modellen die bestudeerd worden door Paltridge, Kleidon, Lorenz en vele anderen [151, 98, 86]. Schrijf  $C_R$  als  $T_T$  (de gemiddelde temperatuur van de tropen) en  $C_W/K_{eq}$  als  $T_P$  (de gemiddelde temperatuur van de polen).  $\kappa^\times$  is nu de snelheidsparameter van het atmosferisch en oceanisch warmtetransport. Deze factor hangt af van de complexe globale circulatieprocessen, dus deze 'effectieve' parameter is enkel goed gedefinieerd indien de atmosfeer in een quasistationaire toestand is (de gemiddelde verdeling van alle eddywervelingen is constant).  $C_R^0$  en  $C_W^0/K_{eq}$  zijn nu de temperaturen die de tropen en de polen zouden bereiken indien er geen warmtetransport van tropen naar polen zou plaatsvinden (dus wanneer  $\kappa^\times = 0$ ).

Deze eenvoudige analogie heeft misschien een hoogst niet-triviaal gevolg. De bovenvermelde klimaatstudies, toegepast op verschillende planeten, formuleren een 'maximum entropieproductie' (MaxEP) hypothese. Indien het voedsel en het afval van het ecosysteem gegeven zijn door ideale oplossingen of gassen, dan kunnen we aantonen dat de entropieproductie (EP) van het ecosysteemmetabolisme in de volledige stationaire toestand (aangeduid met superscript  $*$ ) wordt gegeven door

$$\sigma_{EM}^* = \kappa^* \left( C_R^* - \frac{C_W^*}{K_{eq}} \right) \ln \frac{K_{eq} C_R^*}{C_W^*}. \quad (C.3)$$

In deze stationaire toestand zijn  $C_R^*$  en  $C_W^*$  constant en functies van de drie constante parameters  $\kappa^*$ ,  $\alpha_R$  en  $\alpha_W$ . Plotten we  $\sigma_{EM}^*$  in functie van  $\kappa^*$ , dan zien we dat er een speciale waarde  $\kappa_{MaxEP}^*$  is waarvoor de EP maximaal is (fig. 1.5). De hypothese luidt nu dat de experimentele waarde van  $\kappa^*$  op of dicht bij de MaxEP-waarde ligt. Volgens Paltridge en anderen is er een indicatie dat een dergelijke hypothese werkt voor planetaire klimaatsystemen. Daar het niet de totale EP van het model universum, maar enkel een partiële EP is geassocieerd met het systeem, hebben we dit de '*partiële, stationaire toestand MaxEP*'-hypothese genoemd, om het te onderscheiden van andere MaxEP-hypothesen en principes.

Laten we vervolgens kijken naar een minder complexe schaal: de laminaire stroming of een rudimentair voedsel-consument-voedselweb. Dat laatste voedselweb heeft één additionele variabele, de biomassaconcentratie  $C_C$  van de consument-organismen. Het ecosysteemmetabolisme kan nu geschreven worden als de som van een abiotische conversieterm en een biotische conversieterm die lineair is in  $C_C$ :

$$\kappa_{EM} = \kappa_{AC} + g_{CR}C_C. \quad (C.4)$$

$g_{CR}$  is de voedselopname of groeisnelheid van de consument die zich voedt met het voedsel. De dynamica van de consumenten wordt nu gegeven door de biomassagroei (met een efficiëntiefactor  $q_{CR} \leq 1$ ) min de biomassasterfte (met mortaliteitsparameter  $d_C$ ):

$$\frac{dC_C}{dt} = q_{CR}g_{CR}C_C(C_R - C_W/K_{eq}) - d_C C_C. \quad (C.5)$$

Deze vergelijking, samen met (C.1), vormt een tamelijk 'universele' dynamica, want ons meest intrigerende resultaat toont aan dat deze dynamica perfect kan vertaald worden naar vereenvoudigde dynamische vergelijkingen voor Rayleigh-Bénard convectieve vloeistofcellen (op voorwaarde dat we de limiet  $\alpha_W \rightarrow \infty$  en  $C_W \approx C_W^0$  nemen).

Bovenstaande ecosysteemmodel heeft een speciale eigenschap: introduceren we verschillende soorten consumenten, dan zullen alle soorten uitsterven, behalve de soort met de hoogste overlevingswaarde, gegeven door  $q_{CR}g_{CR}/d_C$ . Dit '*competitieve exclusieprincipe*' kunnen we vertalen naar het vloeistofsysteem om aan te tonen dat die convectiecellen overleven waarvoor de breedte  $\sqrt{2}$  keer de hoogte is.

Tot slot willen we een ecosysteemmodel bespreken dat kan gebruikt worden om verschillende intrigerende vragen m.b.t. de EP van ecosystemen te beantwoorden. We hebben immers een eenvoudige vergelijking voor de totale EP (de EP van het metabolisme plus de uitwisseling met de omgeving) in de stationaire toestand

$$\sigma_{tot}^* = \kappa^* \left( C_R^* - \frac{C_W^*}{K_{eq}} \right) \ln \frac{K_{eq}C_R^0}{C_W^0}. \quad (C.6)$$

De vragen die we willen beantwoorden zijn:

- Heeft de meest stabiele stationaire toestand een hogere EP dan de andere stationaire toestanden? (Deze vraag houdt verband met een '*niet-variationeel MaxEP*' hypothese, niet te verwarren met de partiële stationaire toestand MaxEP.)

- Stijgt de EP als het systeem verder uit evenwicht wordt gedreven? Het externe concentratieverschil  $C_R^0 - C_W^0/K_{eq}$  kan dienst doen als maat voor de afstand van thermodynamisch evenwicht. (Deze vraag houdt verband met het werk van Kay en Schneider [179].)
- Heeft een levend ecosysteem een hogere EP dan een dood ecosysteem bij dezelfde randvoorwaarden? Met andere woorden: zijn biotische processen irreversibeler dan abiotische bij eenzelfde  $C_R^0 - C_W^0/K_{eq}$ ? (Deze vraag houdt verband met de hypothese van Ulanowicz en Hannon [199].)
- Stijgt de EP onder ecosysteemevolutie (door mutatie, immigratie en natuurlijke selectie)?

Laten we eens kijken naar een Lotka-Volterra-chemostat-model met één voedselbron, één consument en één omnivoor, en met een biotische limitatie op instroom van voedsel. De dynamica van dit model is gegeven door:

$$\begin{aligned} \frac{d}{dt}C_R &= (\alpha_R - l_C C_C - l_O C_O)(C_R^0 - C_R) \\ &\quad - (\kappa_{AC} + g_{CR} C_C + g_{OR} C_O)(C_R - C_W^0/K_{eq}) \\ &\quad + d_C C_C + d_O C_O, \end{aligned} \quad (C.7)$$

$$\frac{d}{dt}C_C = q_{CR} g_{CR} (C_R - C_W^0/K_{eq}) C_C - g_{OC} C_C C_O - d_C C_C, \quad (C.8)$$

$$\frac{d}{dt}C_O = q_{OC} g_{OC} C_C C_O + q_{OR} g_{OR} (C_R - C_W^0/K_{eq}) C_O - d_O C_O, \quad (C.9)$$

met  $l_b$  de biotische instroom limitatie parameters,  $g_{bb'}$  de groeiparameters (van  $b$  die  $b'$  consumeert),  $q_{bb'} \leq 1$  de groei-efficiënties en  $d_b$  de sterfteparameters.

Berekenen we nu de stationaire toestand, en daaruit de EP  $\sigma_{tot}^*$ , dan kunnen we parameters kiezen (die a priori niet onmogelijk zijn, dus geen negatieve parameters bijvoorbeeld) zodat elke vraag met een "nee" moet worden beantwoord. Zie fig. 1.6 voor een kwalitatief gedrag van  $\sigma_{tot}^*$  in functie van  $C_R^0 - C_W^0/K_{eq}$ .

Merk op dat de stationaire toestanden van dit model niet overeenstemmen met de partiële stationaire toestand MaxEP-hypothese. Dit ecosysteem is misschien te eenvoudig. Een nieuwe hypothese kan luiden dat een realistischer, complexer voedselweb overeenstemt met een complex, turbulent vloeistof- of klimaatsysteem, en dat bijgevolg realistische ecosystemen wel MaxEP kunnen vertonen. Echter, er is nog geen voldoende verklaring of experimentele observatie om dat te bevestigen.

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