Thermodynamics as a Substantive and Formal Theory for the Analysis of Economic and Biological Systems

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THERMODYNAMICS AS A SUBSTANTIVE AND FORMAL THEORY FOR THE ANALYSIS OF ECONOMIC AND BIOLOGICAL SYSTEMS

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door

Tânia Alexandra dos Santos Costa e Sousa

geboren te Beira, Mozambique

promotor: prof.dr. S.A.L.M. Kooijman

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Chapter 1

Introduction

In this dissertation, we use thermodynamic theory to analyse economic and biological systems, according to two methodological approaches. Substantive integration is a methodological approach that consists of making two different fields compatible, e.g., thermodynamics and biology or thermodynamics and economics, either by reformulating current theories or by building up new theory [6, 14]. For example, theories that explain and describe economic and biological systems must be compatible with thermodynamics because thermodynamic laws impose constraints on mass, energy and entropy flows. A formal analogy is a methodological approach of developing an isomorphism between the mathematical formalisms of different fields [6, 14]. For example, thermodynamics has a solid mathematical formal structure that describes equilibrium, non-equilibrium and self-organized systems that provides a possible common framework to describe thermodynamic, biological and economic systems.

In this dissertation, we concentrate 1) on the substantive integration between thermodynamics and biological systems, 2) on the formal analogy between thermodynamics and economic systems and 3) on the formalization of the Dynamic Energy Budget (DEB) Theory - a theory for biological systems as a prelude to a formal analogy between economic and biological systems.

In a formal analogy between thermodynamic, biological and economic systems, a mathematical framework is developed that simultaneously describes these systems. Formal analogies are important because 1) they reduce the number of logical reasonings used in the different fields of knowledge, 2) they provide a similar interpretation for different phenomena and 3) the knowledge that exists in one field is transposed to another contributing to new developments. However, formal analogies have to be done with great care identifying whether the conditions that have to be met in the original field of knowledge are also met in the field where the analogy is taken. In this dissertation, an isomorphism is established between equilibrium macroscopic thermodynamics and neoclassical microeconomics using a mathematical framework based on the Gibbs-Tisza-Callen approach to equilibrium thermodynamics [2, 4, 19].

Equilibrium thermodynamics characterizes a macroscopic system that evolves in such a way that some thermodynamic potential is optimized. The existence of this extremum keeps the system stable because, when some fluctuation drives the system away from equilibrium, the optimization behaviour brings it back [12]. Neoclassical microeconomics describes the consumer maximizing his utility or the firm maximizing its profit. We focus on the neoclassical microeconomic description of the consumer's behavior because it is the standard theory used to describe the behavior of firms and consumers [15, 22].

In a substantive integration, thermodynamic laws are applied to economic and biological processes to obtain the constraints imposed on the relations between inputs, outputs and the system's state. Also, new theory compatible with thermodynamics can be developed to describe economic and biological processes. Substantive integrations are important because they contribute to the external coherence between different different domains. In this dissertation, non-equilibrium thermodynamics [5, 8, 12, 16, 18], is used to make a substantive integration with biological systems.

Non-equilibrium thermodynamics should be used as a substantive theory because economic and biological systems are open thermodynamic systems kept out of thermodynamic equilibrium due to mass and energy flows. In this work, we take further the substantive integration between the most general framework of non-equilibrium thermodynamics and an organism described by the Dynamic Energy Budget (DEB) theory.

DEB theory describes the way organisms acquire and use matter and energy [13] linking all levels of organization, from membrane physiology to ecosystem dynamics. We use DEB theory to describe biological systems because 1) it has been successfully tested for many organisms including bacteria, yeasts, unicellular algae, lichens, fishes, nematodes, birds and mammals, 2) it is applicable to all species and 3) it is based on the description of mass and energy flows. In this dissertation, we build an axiomatic formalism to describe metabolism that is fully compatible with DEB theory. This formalization of DEB theory and the steps taken in the substantive integration between non-equilibrium thermodynamics and DEB theory facilitate the development of new economic theory compatible with thermodynamics by later establishing an analogy between economic and biological systems.

A good example to ilustrate the simultaneous existence of a substantive integration between the firm and thermodynamics and of a formal analogy between the firm and the organism is the field of industrial metabolism. In this field, there is a substantive integration because economic flows, i.e., the whole integrated collection of physical processes that convert raw materials and energy, plus labour, into finished products and wastes, are described as mass and energy flows [1] and there is a formal analogy because the firm is considered to be the economic analogue of a living organism [1].

Outline of the Dissertation

This dissertation comprises four chapters. Chapter 2 explores the formal analogy between microeconomics and equilibrium thermodynamics. Here, we show that neoclassical microeconomics is formally analogous to equilibrium thermodynamics proving that neoclassical economics has irreversibility embedded in it and we obtain a definition of irreversibility in economic behavior.

Chapter 3 is an elaboration on chapter 2. Here, the isomorphism between thermodynamics and economics is taken much further including the definition of Legendre transforms, Maxwell relations, Le Chatelier Principle and first order phase transitions in economic systems. The equivalence between variables used in microeconomics and thermodynamics is established, new results are obtained in both fields and the differences between the two optimization problems are systematized.

Chapter 4 addresses the substantive integration between thermodynamics and biology. Here, non-equilibrium thermodynamics is applied to an organism that follows the rules of DEB theory. Results include thermodynamic constraints on the behaviour and on the thermodynamic properties of aerobic and non-aerobic organisms. DEB's concept of reserve density is shown to be crucial in discussions concerning entropy production in organisms.

Chapter 5 formalizes into assumptions and propositions DEB theory and links it in a precise way with the empirical patterns that characterize metabolism. This formalization makes it easier to discuss the consequences of alternative metabolic theories. Results also include an alternative proof of a crucial concept in DEB theory and a novel way to present DEB's theory on parameter values.

In this dissertation, we have concluded that:

- The existence of a formal analogy does not imply a substantive integration and vice-versa. This is evident in the relation between thermodynamics and microeconomics: a formal analogy between the two does not mean that microeconomic theory is compatible with thermodynamic laws.

- Formal analogies contribute to the solution of problems that exist in the theoretical structure of a scientific discipline. For example, the discussion on whether the microeconomic formalism has irreversibility embedded in it is clarified by the isomorphism established in chapter 2.
- Formal analogies contribute to obtain new results in a discipline. For example, the relationship between elasticities in economics and the distinction between mathematical integrability and optimization behaviour in thermodynamics.
- The identification of an isomorphism between two or more different disciplines simplifies the learning process. A clear example is presented in chapter 3 where the concept of economic integrability is shown to be equivalent to the Generalized Le Chatelier Principle.
- The substantive integration between thermodynamics and other disciplines contributes to new results about the systems studied. For example, in chapter 4 we obtain the result that anaerobic organisms have a higher flexibility in their thermodynamic behaviour.

Outlook

We used equilibrium thermodynamics to build up a formal analogy with one consumer in chapters 2 and 3. The formal analogy can be extended to a profit maximizing firm or to a social welfare maximizing central planner. Equilibrium thermodynamics can also be used to establish a formal analogy with the optimal foraging strategy in ecology [21].

The transition from maximizing utility to maximizing social welfare is not straightforward because the equilibrium states that result from multiple optimizing agents are different from the equilibrium state that results from an aggregate optimizing function. The set of conditions under which optimizing consumers and producers lead to the maximization of social welfare is a crucial issue in economics [10]. The same issue can be raised in ecological systems about the relation between optimizing organisms and the optimization of an ecosystem [11].

Statistical physics [9, 20] explains the macro thermodynamic behavior by imposing a probability distribution over the microscopic dynamical states. This paradigm would be useful as a formal tool to explore the relationships between different scales in economic and ecological systems. Also, the scaling up from microeconomic systems to macroeconomic systems that is achieved by using the equilibrium results at the micro scale to build models at the macro scale [17] can be applied to ecological systems.

In this dissertation, we do not use the formal structure that describes the evolution of thermodynamic systems from equilibrium, to non-equilibrium and self-organization. The dynamics of systems out of equilibrium, but close to equilibrium, is characterized by linear equations [2, 5, 12]. In these linear nonequilibrium thermodynamic systems (LNET) the production of irreversibilities is minimized. The dynamics of systems far away from equilibrium, studied in the framework of extended nonequilibrium thermodynamic systems (ENET), is characterized by nonlinear equations [12]. These far away from equilibrium systems are created and maintained by dissipative processes and evolve unpredictably with some of these possible final states being states that possess spatiotemporal organization [12]. This formal structure can be applied to economic and ecological systems to help characterize the evolution path for ecosystems and for economies [7].

The logical structure developed by Clausius-Kelvin-Carathéodory to describe equilibrium thermodynamics [19] can be used to establish a formal analogy with economics instead of the approach of Gibbs-Tisza-Callen used in this dissertation. A formal relationship between the two approaches to thermodynamics is already established [4, 19].

We use non-equilibrium thermodynamics to make a substantive analogy with the organism described by the Dynamic Energy Budget Theory in chapter 4. Although the main target of DEB theory is the organism, it also establishes links to the cellular and food web levels [13]. This means that DEB theory can be used together with non-equilibrium thermodynamics to extend the substantive integration to the cellular, organismic and ecological levels.

We formalize DEB theory into assumptions and propositions in chapter 5. This is a first step to use DEB theory to build up a non-optimizing theory in economics that would describe in more realistic terms the behavior of consumers and firms and at a more aggregate level the wealth of a country. This would also be an intermediate step for a substantive integration between thermodynamics and economics because DEB is compatible with non-equilibrium thermodynamics.

A description of both economic and ecological systems that is compatible with non-equilibrium thermodynamics is a crucial step to determine one of the most important issues in the interaction between ecologic and economic systems: the maximum scale of economic systems [3].

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Chapter 2

Is neoclassical economics formally valid? An approach based on an analogy between Equilibrium Thermodynamics and Neoclassical Microeconomics

Abstract

The relation between Thermodynamics and Economics is a paramount issue in Ecological Economics. Two different levels can be distinguished when discussing it: formal and substantive. At the formal level, a mathematical framework is used to describe both thermodynamic and economic systems. At the substantive level, thermodynamic laws are applied to economic processes.

In Ecological Economics, there is a widespread claim that neoclassical economics has the same mathematical formulation as classical mechanics and is therefore fundamentally flawed because: 1) utility does not obey a conservation law as energy does; 2) an equilibrium theory cannot be used to study irreversible processes. Here, we show that neoclassical economics is based on a wrong formulation of classical mechanics, being in fact formally analogous to equilibrium thermodynamics. The similarity between both formalisms, namely that they are both cases of constrained optimisation, is easily perceived when thermodynamics is looked upon using the Tisza-Callen axiomatisation. In this paper, we take the formal analogy between equilibrium thermodynamics and economic systems far enough to answer the formal criticisms, proving that the formalism of neoclassical economics has irreversibility embedded in it.

However, the formal similarity between equilibrium thermodynamics and neoclassical microeconomics does not mean that economic models are in accordance with mass, energy and entropy balance equations. In fact, neoclassical theory suffers from flaws in the substantive integration with thermodynamic laws as has already been fully demonstrated by valuable work done by ecological economists in this field.

Keywords: Thermodynamics, Entropy, Neoclassical Economics, Analogy and Irreversibility.

2.1 Introduction

The relation between Thermodynamics and Economics is a paramount issue in Ecological Economics. Two different levels can be distinguished when discussing it: formal and substantive.

At the formal level, a mathematical framework is used to describe both thermodynamic and economic systems. This allows for insights that were gained in one field of knowledge to be transposed to another. However, this has to be done with great care identifying whether the conditions that have to be met in the original field are also met in the field where the analogy is taken.

At the substantive level, thermodynamic laws are applied to economic processes. The integration between economics and thermodynamics at the substantive level is of crucial importance because economic processes obey thermodynamic laws and therefore a sound economic theory must be coherent with thermodynamics. This integration highlights the dependence between the economic system and the biophysical framework contributing to the analysis of the sustainability of economic systems.

This distinction between formal analogy and substantive integration is not a new issue, e.g., Martinez-Alier [33] says that ‘the mathematical description of economic phenomena in the language of physics is different from applying the concepts of physics’. Also, Baumgärtner [9] discussing the different ways in which thermodynamics can be incorporated in economic analysis, considers the isomorphism of formal structure and the thermodynamic constraints on economic action among others, which are respectively, the formal analogy and the substantive integration discussed in this chapter.

The belief that neoclassical economics is based on a formal analogy to classical mechanics is common among ecological economists. For example, Amir [2] argues that ‘most physical analogies in economic theory are borrowed from mechanics’, Martinez-Alier [33] argues that ‘economic science has used the mathematics of mechanics since the first neoclassical economists' and Costanza et al. [18] say that 'the market model has been formalized using the same mathematics as used by Newton for mechanical systems'. Outside ecological economics, this thesis has been most extensively argued by Mirowski [34], who considers that neoclassical economics is an attempt to emulate classical mechanics.

Based on this supposed analogy to classical mechanics, the main formal criticisms of neoclassical economics are: utility does not obey a conservation law as energy does; an equilibrium theory cannot be used to study irreversible processes.

Here, we argue that neoclassical economics is not formally identical to classical mechanics and that the correct identification of the formalism that underlies the construction of neoclassical economics is vital in the evaluation of its internal coherence. We show that economics is formally identical to thermodynamics because they are both problems of static constrained optimisation. The similarity between both formalisms has already been explored in the literature since the 40' [22, 30, 40, 41] and more recently [1, 12, 15, 16, 43, 44, 49, 50].

The formal analogies of Saslow [43], Berry et al. [12] and Amel'kin et al. [1] are driven from superficial similarities between the entities of economy and thermodynamics instead of being derived from fundamental principles. Therefore, these analogies are not helpful in answering the criticisms raised by ecological economists concerning the formal coherence of economic theory.

Candeal et al. [15, 16] prove that the mathematical representations of entropy and utility are analogous. Candeal et al. [15] and Cooper [17] investigate the mathematical foundations of the entropy representation where the entropy is built as an order preserving function that satisfies a continuity property. Candeal et al. [16] establish a formal relation between the entropy function and the utility function for the axioms that establish the existence of both ordering functions. Although, these authors do not develop their analysis any further, the formal analogy obtained at the function level is important and it lies behind the optimisation analogy pursued here.

The claim that neoclassical economics is formally identical to classical mechanics has also led many Ecological Economists to the substantive assertion that neoclassical economics is fundamentally flawed because it ignores thermodynamics. This argument lacks coherence because the existence of a formal analogy does not imply the existence of a substantive integration and vice-versa. This statement about the non-equivalence between the formal analogy and the substantive integration is easily argued, in this case, because the formal analogy uses the entities that are part of economic theory, i.e., utility, while the substantive integration uses the mass, energy and entropy flows in economic systems.

Another argument that should help clarifying this issue is that different physical phenomena are described with different mathematical formalisms although they all have to obey thermodynamic laws. Whether neoclassical economics is formally identical to classical mechanics is not straightforwardly related to its substantive relation with thermodynamic laws.

For the same reason, although here we show that neoclassical economics is formally identical to thermodynamics, this does not imply that it is substantively compatible with thermodynamic laws. Whether neoclassical economics is in agreement with thermodynamic laws should be evaluated by looking at the 'entropic flow of energy and materials that runs through the economy' [33] instead of being based on the use of formal arguments. We would like to emphasize that ecological economics has already given many important contributions to this substantive integration between thermodynamics and economics with, among many others, the works of Georgescu-Roegen [25], Daly [19], Biancardi et al. [13], Ruth [38, 39], Stern [46], Ayres [4, 5, 6], Baumgärtner et al.[11], Ayres et al. [7], Tiezzi [47] and Frondel and Schmidt [24].

The roadmap of this chapter is as follows. In section 2.2, we motivate the reader for our formal analogy: (1) by explaining why there is the widespread idea that neoclassical economics is formally analogous to classical mechanics and (2) by reviewing some of the incorrect formal criticisms of neoclassical economics. In section 2.3, we present a unified formalism for thermodynamic and economic systems, based on the formalism of constrained optimisation. In section 2.4, some of the formalism's characteristics, namely its limits and scope and other related issues, are clarified. Section 2.5 concludes and argues that although there is a formal analogy between thermodynamics and neoclassical economics, these two fields are not substantively compatible.

2.2 Is the Formalism of Neoclassical Economics wrong?

It is generally claimed that neoclassical economics is based on classical mechanics because throughout the history of economics many economists used analogies from classical mechanics. Mirowski [34] gives some examples of the use of mechanical concepts and metaphors: (1) the lever rule by Nicolas Canard, (2) gravitation theory by Stanley Jevons, (3) force by Herman Gössen, (4) power by Frederick Soddy and (5) the Energy Minimum Principle by Francis Edgeworth.

This approach of establishing analogies between mechanics and economics was taken to its extreme by Irving Fisher who in 1892 established the most extensive relation between mechanics and economics (Table 2.2). According to Fisher [23], while economic equilibrium corresponds to maximum profit, mechanical equilibrium corresponds to minimum energy.

Mechanics	**Economics**
Particle	Individual
Space^{*1}	Commodity^{*1}
Force^{*1}	MU^{*1}
Work = force · space^{*2}	Disutility = MU · commodity^{*2}
Energy = force · space^{*2}	Utility = MU · commodity^{*2}
Equilibrium: impelling and resisting forces along each axis are equal	Equilibrium: MU and marginal disutility along each axis are equal

Table 2.1: The analogy between mechanics and economics proposed by Fisher (1991, p. 85). ^{*1} (vector), ^{*2} (scalar) and MU(marginal Utility).

Given the history of economic analogies to mechanics, there is a widespread claim that neoclassical economics is fundamentally flawed because the assumptions on which classical mechanics is based do not apply to consumer theory. The most important aspects usually referred in the literature are: 1) utility does not obey a conservation law as energy does; 2) an equilibrium theory cannot be used to study irreversible processes. Some of the examples of this are described below.

Mirowski [34] considers that ‘forgetting the conservation of energy while simultaneously appealing to the metaphor of energy ... is the Achilles heel of all neoclassical economics’ because, according to Mirowski, although utility cannot be a conserved entity, the results obtained in consumer theory assume that it is.

Amir [2, 3] claims that the utility function is unlikely to be a conserved quantity, but that economic theory assumes that it is, which is supposedly patent in the use of the proportionality between marginal utilities and market prices in equilibrium.

Georgescu-Roegen [25] argues that Jevons and Walras, whose aim was to create an economic science similar to mechanics, built an economic theory that only describes reversible and qualityless motion. Georgescu-Roegen also argues that ‘economics...is mechanistic in the same strong sense...[that] classical mechanics...because neither induces any qualitative change nor is affected by the qualitative change of the environment’.

Lozada [31] states that the entropy law is not reducible to mechanics by saying that ‘the inconsistency between the logical structure of the entropy law and the logical structure of neoclassical economic analysis is that the former is evolutionary and the other is arithmomorphic and hence non-evolutionary'.

However it is important to emphasize that some authors do disagree with the supposed analogy between classical mechanics and neoclassical economics, e.g., Varian [51], in a review of Mirowski's book, argues that if the energy conservation principle implies that utility is not a coherent concept then this implies that utility is not energy', Marchionatti and Gambino [32] say that 'a critique, such as that of Mirowski, of the mechanical analogy in neoclassical economics, seems largely unhelpful and based on a misunderstanding' and Hands [27] argues that the standard Slutsky conditions, that are sufficient for the integrability of demand, do not seem to be sufficient to guarantee, as Mirowski argues, that prices form a conservative vector field.

We agree that if neoclassical economics were indeed formally identical to classical mechanics it would be internally incoherent. However, we argue that neoclassical economics is based on a wrong formulation of classical mechanics, being in fact formally identical to thermodynamics. Both neoclassical economics and thermodynamics are equilibrium theories and can be developed as formalisms of constrained optimisation as shown in the next section.

2.3 A Unified Formalism for Neoclassical Economics and Equilibrium Thermodynamics

In this section, a mathematical unified formalism based on the axiomatization of Tisza-Callen is first developed in the general case and then applied to thermodynamic and to economic systems.

2.3.1 General Formalism

The constrained optimisation problem describes the behaviour of the system that evolves in order to maximize some function y subject to a set of constraints[1]. In equilibrium the values acquired by the variables, x_i, $i = 1,\dots,n$, maximize the potential y, given the constraints.

This maximization is constrained because the variables in equilibrium have to obey a set of constraints, $g_z = 0$, $z = 1,\dots,m$. These constraints are a function of the initial values

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[1] Minimization is an equivalent problem.

of the variables, x_i^0, and of some parameters k_j, j=1,. . . ,l:

$$\max_{x_1,\dots,x_n} \quad y\left(x_1,\dots,x_n\right) \quad s.t.\ g_z\left(x_1,\dots,x_n,x_1^0,\dots,x_n^0,k_1,...,k_l\right)=0. \tag{2.1}$$

This problem is solved with the Method of Lagrangean Multipliers[2]. The Lagrangean function, L, is defined as:

$$\begin{gathered} L\left(x_1,...,x_n,k_1,...,k_l,\lambda_1,...,\lambda_m\right)= \\ y\left(x_1,...,x_n\right)+\sum_{z=1}^{m}\lambda_z g_z\left(x_1,...,x_n,x_1^0,...,x_n^0,k_1,...,k_l\right). \end{gathered} \tag{2.2}$$

The values of the variables that maximize the objective function subject to the constraints are obtained solving the system of $m+n$ equations:

$$\begin{aligned} \frac{\partial L}{\partial x_i} &= 0,\ i=1,...,n, \\ \frac{\partial L}{\partial \lambda_z} &= 0,\ \mathrm{z}=1,...,m \end{aligned}$$

which is equivalent to:

$$\begin{aligned} \frac{\partial y}{\partial x_i} &= -\sum_{z=1}^{n}\lambda_z\frac{\partial g_z}{\partial x_i},\ i=1,...,n \\ g_z &= 0,\ \mathrm{z}=1,...,m \end{aligned} \tag{2.3}$$

If the function y and the constraints g_z are real valued and differentiable, if the number of constraints, m, is less than the number of variables, n, and if the gradient vectors of the constraint equations are linearly independent, the maximum exists. In this case, Lagrange's Method gives the first order equilibrium conditions [28], Eq. 2.3, which define the state of the system. These equilibrium conditions give the optimal values of each x_i, x_i^*, as a function of the parameters k_j and of the initial conditions:

$$x_i^*=f\left(k_1,...,k_l,x_1^0,...,x_n^0\right). \tag{2.4}$$

With the set of equations (2.4) the optimal value of y, y^*, can also be written as:

$$y^*=f\left(k_1,\dots,k_l,x_1^0,...,x_n^0\right). \tag{2.5}$$

In the initial state, the system is characterized by the values x_i^0; which are called initial conditions. In the final state, the system is characterized by the optimal values assumed

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[2] For a more detailed description of this method see, e.g., Jehle (1991).

by the variables, x_i^*. The evolution of the system from the initial to the final state is called a process. In a reversible process, the initial and final states have the same y^*. In an irreversible process, the final state has a higher value of y^* than the initial state. The amount of irreversibility (always positive) produced in an irreversible process can be measured by the increase in y. An impossible process is a process that will never occur because if it did the final state would have a lower value of y^*.

2.3.2 Thermodynamic Systems

The constrained optimisation problem in thermodynamics is the maximization of the entropy of a composite system with constant total internal energy, constant total volume and constant total mole numbers.

The entropy of a homogeneous thermodynamic system can be obtained from the fundamental equation [48, 14] [3]:

$$S = S\left(U, V, N\right). \tag{2.6}$$

The variables are S, the entropy, U, the internal energy, V, the volume, and $N$the number of moles.

The problem of the maximization of entropy for a composite system[4] comprising two simple systems (1 and 2) is formalized as[5]:

$$\max_{U_1,U_2,V_1,V_2,N_1,N_2} S = S_1\left(U_1, V_1, N_1\right) + S_2\left(U_2, V_2, N_2\right),$$

s. t.

$$\begin{aligned} U_1 + U_2 &= U_1^0 + U_2^0 \\ V_1 + V_2 &= V_1^0 + V_2^0 \\ N_1 + N_2 &= N_1^0 + N_2^0 \end{aligned} \tag{2.7}$$

where the constraints are that, over the two systems, the sums of the internal energies, the mole numbers and the volumes are kept constant. The initial conditions are the internal energy U_j^0, the mole numbers N_j^0 and the volume V_j^0 for *j*= 1,2.

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[3] Where, for simplicity, we consider a system with a single chemical component.

[4] Carathéodory introduced the concept of composite systems because the entropy is axiomatically only defined for equilibrium systems.

[5] For simplicity, we consider only two subsystems.

Defining temperature, T_j, pressure, P_j, and chemical potential, μ_j, for j= 1,2, as:

$$\begin{aligned}\frac{\partial S_j}{\partial U_j} &\equiv \frac{1}{T_j} \\ \frac{\partial S_j}{\partial V_j} &\equiv \frac{P_j}{T_j} \\ -\frac{\partial S_j}{\partial N_j} &\equiv \frac{\mu_j}{T_j}\end{aligned} \tag{2.8}$$

with $S_j = S_j(U_j{,}V_j{,}N_j)$, j= 1,2, the equilibrium conditions, see Eq. 2.3, for the thermodynamic system subject to the previous constraints are:

$$\begin{aligned}\frac{1}{T_1} &= \frac{1}{T_2} \\ \frac{P_1}{T_1} &= \frac{P_2}{T_2} \\ \frac{\mu_1}{T_1} &= \frac{\mu_2}{T_2}\end{aligned}$$

. That is, equilibrium is established when both systems have the same temperature, the same chemical potentials and the same pressure. Thus, an isolated composite system whose constraints are defined above increases its entropy towards the maximum value by turning into a system with a homogeneous temperature, homogeneous pressure and homogeneous chemical potential.

These equilibrium conditions are also explainable by reductio ad absurdum. Suppose that, in the equilibrium state, the temperatures of the two systems were not equal, e.g., $\mathrm{T}_1 > \mathrm{T}_2$. If energy would flow (in the form of heat) from system 1 to system 2, system 2 would increase its entropy and system 1 would decrease its entropy because the derivative of the entropy in relation with energy, Eq. 2.8, is always positive given that the absolute temperature is always positive. The increase in entropy of system 2 would be higher than the decrease in entropy of the other system because its temperature is lower, again by Eq. 2.8. Therefore, the global change in entropy would be positive and consequently the initial equilibrium state did not have the highest entropy possible, which means it was not an equilibrium state.

Each optimal variable, see Eq. 2.4, can be written as:

$$\begin{aligned}U_j^* &= f\left(V_1^0, V_2^0, U_1^0, U_2^0, N_1^0, N_2^0\right), j = 1, 2, \\ N_j^* &= f\left(V_1^0, V_2^0, U_1^0, U_2^0, N_1^0, N_2^0\right), j = 1, 2 \\ V_j^* &= f\left(V_1^0, V_2^0, U_1^0, U_2^0, N_1^0, N_2^0\right), j = 1, 2,\end{aligned} \tag{2.9}$$

These equations give the optimal value of the variables of each system as a function of the initial conditions. The maximum entropy, see Eq. 2.5, as a function of the same arguments is:

$$S^{*} \quad = \quad f\left(V_1^0, V_2^0, U_1^0, U_2^0, N_1^0, N_2^0\right). \tag{2.10}$$

Reversible processes in a thermodynamic system are processes that occur in an isolated system at constant maximal entropy. Impossible processes are processes that do not occur because the isolated system would decrease its maximum entropy. Irreversible processes in a thermodynamic system are processes that occur in an isolated system at increasing maximal entropy. The amount of irreversibility produced is equal to the variation in entropy between the initial state and the equilibrium state.

2.3.3 Consumer System

The extremum principle, in consumer theory, is the maximization of utility of a consumer at constant market prices and constant endowment. When allowed to trade with the market, the consumer maximizes his utility, U.

The consumer's utility maximization problem is

$$\max_{x_1,\ldots,x_n} U = U\left(x_1,\ldots,x_n\right)$$

s.t.

$$p_1x_1 + \ldots + p_nx_n = p_1x_1^0 + \ldots + p_nx_n^0. \tag{2.11}$$

where the constraint is that the total cost of goods that will be bought (left hand side of the constraint) is equal to his initial endowment $p_1x_1^0$ +...+$p_nx_n^0$. The variables are the different amounts of goods, x_i, the parameters are the market price p_i of good i, i = $1,\ldots, n$. The initial conditions are the amounts of each good i in the initial state, x_i^0.

Defining marginal utilities as:

$$\frac{\partial U}{\partial x_i} \equiv MU_i, \quad i = 1,\ldots,n, \tag{2.12}$$

with $U = U(x_1,\ldots,x_n)$, the equilibrium conditions, see Eq. 2.3, for the consumer are:

$$\frac{MU_1}{p_1} = \ldots = \frac{MU_n}{p_n}.$$

A consumer system whose constraints are that the endowment and the prices remain constant increases his utility towards the maximum value by exchanging with the market until the ratio between marginal utility and price is the same for all products.

Varian [52] proves this optimum condition by reductio ad absurdum using the following argument. Suppose that the consumer's utility is maximum but that the ratio between marginal utilities of product i and product j is two and the ratio of prices is one. Then, the consumer will exchange one unit of product j for one unit of product i obeying the endowment constraint (they are worth the same) and increase his utility. This means that the initial state was not at the maximum utility.

Each optimal value, see Eq. 2.4, can be written as:

$$x_j^* \quad = \quad f\left(p_1, p_2, ..., p_n, x_1^0, ..., x_n^0\right) \quad j = 1, \ldots, n \ . \tag{2.13}$$

These equations give the optimal amount of product j as a function of the prices and initial amounts of each product. The maximum utility as a function of the same arguments is the equilibrium condition analogous to Eq. 2.5,

$$U^* = f\left(p_1, \ldots, p_n, x_1^0, ..., x_n^0\right) . \tag{2.14}$$

Reversible processes for the same consumer are processes in which he trades with the market but does not increase his maximum utility. Impossible processes are trades that do not occur because the consumer would decrease his maximum utility. Irreversible processes for the consumer are processes characterized by an increase in utility: if a consumer engages in a trade that increases his utility, he will not reverse the trade. The amount of irreversibility produced is equal to the amount of utility increase between the initial state and the equilibrium state.[6]

2.4 Discussing the Formalism

In this section we clarify some of the points of the formalism presented.

2.4.1 On the correct thermodynamic framework for substantive integration

We would like to emphasize that the substantive integration between thermodynamics and economic systems should not be based on the thermodynamic theory of isolated systems that we present in this chapter. Economic systems are open thermodynamic systems far from equilibrium and therefore a thermodynamic analysis of economic systems should be based on the thermodynamics of nonequilibrium open systems [29, 37, 35, 36, 26].

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[6] This statement does not mean that we are considering that utility is a cardinal concept. This is further discussed in section 2.4.3.

2.4.2 On the concept of equilibrium

In the formalism of constrained optimization, equilibrium is the extremum point subject to the constraints considered. It is equilibrium because the system will not move from that point unless the constraints are changed. For example, for a certain amount of total internal energy, total volume and total number of moles, a thermodynamic system is in equilibrium if its entropy is at the maximum level (S*). This entropy equilibrium value (S*) can only be changed if the constraints are changed, e.g., the system receives a heat flow from the exterior hence increasing its total energy. The same is applicable to the consumer: for a certain total cost of goods, a consumer system is in equilibrium if its utility is at the maximum level (U*). This utility level (U*) can only be changed if the constraints are changed, e.g., the consumer receives an additional endowment.

The formal equilibrium considered for the consumer problem is not the thermodynamic equilibrium of the consumer. The thermodynamic equilibrium of the consumer would be a dead consumer.

2.4.3 On the ordinal concept of utility

Utility is usually considered in an ordinal framework, i.e, utility functions order the consumption bundles according to the preferences of the consumer but the absolute values of utility have no meaning. This means that if utility function $U(x_1,\ldots,x_n)$, represents the preferences of the consumer, then so does any other utility function obtained through a positive monotonic transformation $U^\theta = f(U(x_1,\ldots,x_n))$, (Jehle, 1991), i.e.,

$$\frac{\partial U^\theta}{\partial U} = \frac{\partial f\left(U\right)}{\partial U} > 0. \tag{2.15}$$

Our proposed formalism does not entail a cardinal concept of utility and is fully compatible with the ordinal framework because (1) the equilibrium conditions obtained and (2) the ranking of the amount of irreversibilities produced are both independent of the specific utility function chosen within the family of monotonic transformations. (1) is proved by Samuelson [42] and (2) is obtained below.

The amount of irreversibility produced between an initial state characterized by $x_1,\ldots,x_n$ and a final equilibrium state $x_1^*,\ldots,x_n^*$ can be measured using the utility function U or any other positive monotonic transformation $U^\theta = f\left(U\right)$:

$$\begin{array}{l} \sigma = U^*\left(x_1^*,\ldots,x_n^*\right) - U\left(x_1,\ldots,x_n\right) \\ \sigma^\theta = U^{\theta *}\left(x_1^*,\ldots,x_n^*\right) - U^\theta\left(x_1,\ldots,x_n\right) \end{array} . \tag{2.16}$$

We prove that σ^θ is a positive monotonic transform of σ, using Eq. 2.15,

$$\frac{\partial \sigma^\theta}{\partial \sigma} = \frac{\partial \left(U^{\theta *}\left(x_1^*, \ldots, x_n^*\right) - U^\theta\left(x_1, \ldots, x_n\right)\right)}{\partial \left(U^*\left(x_1^*, \ldots, x_n^*\right) - U\left(x_1, \ldots, x_n\right)\right)} = \tag{2.17}$$
$$\frac{\partial U^{\theta *}\left(x_1^*, \ldots, x_n^*\right)}{\partial U^*\left(x_1^*, \ldots, x_n^*\right)} + \frac{\partial U^\theta\left(x_1, \ldots, x_n\right)}{\partial U\left(x_1, \ldots, x_n\right)} > 0.$$

Summarizing, the amount of irreversibilities produced between any initial state and the equilibrium state has an ordinal meaning, i.e., if the amount of irreversibilities produced going from state A to equilibrium is higher than the amount of irreversibilities produced going from state B to equilibrium, then the consumer will behave such as to move from state A to state B but not the reverse.

2.5 Conclusions

In the ecological economics literature, the validity of neoclassical economics has been widely discussed. This discussion has not been as fruitful as expected because the distinction between formal and substantive criticisms is blurred in many of the arguments presented.

In this chapter, we present and explore the validity of the formal criticisms of neoclassical economic theory. We concluded that formal criticisms are wrong because they are either based on mixing up the substantive and formal levels [20, 45] or they are based on the wrong assumption that the microeconomic formalism is analogous to the classical mechanics formalism [2, 3, 25, 31, 34].

We have shown that the argument that the neoclassical formalism is wrong because it was built from mechanics, is not valid; in fact, the neoclassical formalism is identical to the Tisza-Callen axiomatization of thermodynamics. For both thermodynamic and economic systems, we have identified the constrained optimisation problems along with the equilibrium conditions. We have proved that the formalism of neoclassical economics does not consider utility to be a conserved entity because it predicts the existence of irreversible processes characterized by increasing utility at constant market prices.

Smith and Foley [44] also present a formal analogy between neoclassical economics and thermodynamics based on constrained optimisation. These authors consider that the main difference between the two fields is that ‘there is no counterpart in physics for the way neoclassical economists attach importance to transformations respecting initial endowments … and there seems to be no counterpart in economics to the importance thermodynamics attaches to reversible transformations.' The first remark is not correct because initial endowments in consumer theory (initial amounts of goods) are similar to the initial extensive parameters characterizing an isolated composite system (volume, internal energy and number of moles). The second remark is not correct because in consumer theory many results are also obtained for reversible transformations, e.g., the compensating and the equivalent variations. In both fields, reversible transformations are just limiting cases of actual transformations but their study is important because they set limits on real transformations.

Finally, it is of fundamental importance that the fact that neoclassical economics is formally identical to thermodynamics does not mean that it is compatible with thermodynamic laws. Examples of flaws in the integration between economic theory and thermodynamic laws already identified are: economic theory considers a circular flow between households and firms without considering the one-way flow that begins with resources and ends with waste [25]; energy and capital are generally not substitutes, as assumed by production functions, but complements [21, 38, 46]; the Inada conditions are inconsistent with mass conservation [8]; and production theory does not fully possess thermodynamic irreversibility [10].

However these flaws do not result from the similarities between the formal structure of economics and mechanics. This misconception, which results from the use of the formal to argue the substantive, is present in many works like Daly [20], Sollner [45] and Geogescu-Roegen [25].

Daly [20] argues that standard economics explains circular flows because they are mechanistic in nature (reversible and qualityless) and that it does not explain the one-way flow of resources into waste because it is irreversible and mechanistic models cannot deal with irreversibility. We have proved that formally standard economics has irreversibility embedded in it; therefore, the fact that standard economics does not explain the physical directionality of economic flows cannot be accounted for by its formal structure.

Sollner [45] considers that the definition of value in economic theory is incompatible with the entropy law because it was taken from neoclassical mechanics. However, to exemplify this formal flaw, Sollner uses substantive arguments analogous to the ones provided by Georgescu-Roegen.

We argue that the flaws in the economic theory, referred by Sollner [45], Daly [20] and Georgescu-Roegen [25] do exist, but the causality relation used to explain these flaws is not correct. These flaws are due to a lack of substantive integration between thermodynamics and economics instead of being rooted in the supposed 'mechanistic' nature of neoclassical economics.

Concluding, we proved that the analogies to classical mechanics used by economists to build up neoclassical economic theory were wrongly formulated and that instead, neoclassical economic theory was built formally analogous to thermodynamics. Additionally, by clarifying the distinction between formal analogy and substantive integration we made clear that although neoclassical economics and thermodynamics are both formalisms of constrained optimisation they are not substantively compatible.

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Chapter 3

Equilibrium Econophysics: A unified formalism for neoclassical economics and equilibrium thermodynamics

Abstract

We develop a unified conceptual and mathematical structure for Equilibrium Econophysics, i.e., the use of concepts and tools of equilibrium thermodynamics in neoclassical microeconomics and vice-versa. Within this conceptual structure the results obtained in microeconomic theory are: (1) the definition of irreversibility in economic behavior, (2) the clarification that the Engel curve and the offer curve are not descriptions of real processes dictated by the maximization of utility for the microeconomic consumer's formalism considered here, (3) the derivation of a relation between elasticities proving that economic elasticities are not all independent, (4) the proof that Giffen goods do not exist in a stable equilibrium, (5) the derivation that 'economic integrability' is equivalent to the Generalized Le Chatelier Principle and (6) the definition of a first order phase transition, i.e., a transition between separate points in the utility function. In thermodynamics the results obtained are: (1) a relation between the non-dimensional isothermal and adiabatic compressibilities and the increase or decrease in the thermodynamic potentials, (2) the distinction between mathematical integrability and optimization behavior and (3) the generalization of the Clapeyron Equation.

Keywords: Econophysics, Entropy, Utility, Optimization and Unification of Knowledge.

3.1 Introduction

A general definition of econophysics is the use of concepts and tools in Economics that were developed in Physics. The state of the art in this field is the use of statistical physics to get new insights into the behavior of financial markets [8, 10, 11, 15, 19, 21, 29, 32, 36, 39]. Here, we focus instead on the similarity between Neoclassical Microeconomics and Equilibrium Thermodynamics. Some similarities between both formalisms have been explored in the literature since the 40's and 60's [9, 16, 24, 23, 25, 27, 26] and more recently [1, 2, 5, 6, 28, 30, 31, 34, 35]. In this chapter, we develop a unified formalism, for both fields, using the Tisza-Callen axiomatization of thermodynamics [4, 33], and take it further, making contributions both to Economics and to Thermodynamics. Also, by formulating both theories with the same mathematical formalism, neoclassical economics becomes accessible to physicists and thermodynamics becomes accessible to economists. This makes this chapter also an interesting pedagogical tool, e.g., in B.Sc. courses in econophysics like the one proposed by Grech [12].

The road-map of this chapter is as follows. All sections start by the description of the general formalism followed by its application to the equilibrium thermodynamic system and then to the consumer. In section 3.2, the fundamental equation, the constraints and the extremum principle that describe the behavior of these systems are explained and the equilibrium conditions are obtained. An alternative formulation to describe the systems' behavior, the duality equation, is presented in section 3.3. The reversible, irreversible and impossible processes undertaken by these systems are clarified in sections 3.4 and 3.5. In section 3.6, adequate descriptions of systems with a special type of constraints are obtained with the Legendre transforms. In section 3.7, the properties that characterize these systems are identified and in section 3.8 the relation between them is established. The stability conditions, i.e., the constraints imposed on the values of the systems' properties by the maximization principle, are presented in section 3.9 and the process that occurs as a result of instability, i.e., the first order phase transition, is explained in section 3.11. The issue of whether the system is described by the constrained optimization formalism developed in the chapter is addressed in section 3.10. Section 3.12 concludes.

The microeconomic formalism of the consumer can contemplate two cases: (1) a consumer who, in each of many periods, chooses between alternative bundles constrained by the same budget and (2) a consumer who, over a short period of time faces a series of opportunities to buy or sell goods at constant endowment; in the first case the bundle is consumed within that period and in the second case the consumption is postponed [20].

In this chapter, we will focus on the second case because: (1) it is more adequate for financial markets, currently the major focus of econophysics and (2) the similarities with the equilibrium thermodynamics systems are more straightforward.

3.2 Fundamental Equation and the Equilibrium State

A system that evolves in order to maximize some function y subject to a set of constraints [1] is described by a constrained optimization problem: in equilibrium the values acquired by the state variables, x_i, i = 1,...,n, maximize the function y, given the constraints. The function $y(x_1, \ldots, x_n)$ is the **fundamental equation** of the system. The state variables are **extensive variables**, i.e., additive variables.

This maximization is constrained because the variables in equilibrium have to obey a set of constraints, which are a function of the initial values of the variables, x_i^0, and of some parameters k_j, j=1,...,l:

$$\begin{aligned} \max_{x_1,\ldots,x_n} \quad & y\left(x_1,\ldots,x_n\right) \quad s.t. \\ g^z\left(x_1,\ldots,x_n,x_1^0,\ldots,x_n^0,k_1,\ldots,k_l\right) &= 0, \\ z &= 1,\ldots,m. \end{aligned} \tag{3.1}$$

This problem is solved with the Method of Lagrangean Multipliers [2]. The Lagrangean function, $\mathcal{L}$, is defined as:

$$\begin{aligned} \mathcal{L}\left(x_1,\ldots,x_n,x_1^0,\ldots,x_n^0,k_1,\ldots,k_l,\lambda_1,\ldots,\lambda_m\right) = \\ y\left(x_1,\ldots,x_n\right) + \\ + \sum_{z=1}^{m} \lambda_z g^z\left(x_1,\ldots,x_n,x_1^0,\ldots,x_n^0,k_1,\ldots,k_l\right). \end{aligned} \tag{3.2}$$

where λ_z are the Lagrangean multipliers.

The values of the variables that maximize the objective function subject to the constraints are obtained solving the system of $m + n$ equations:

$$\frac{\partial \mathcal{L}}{\partial x_i} = 0, \quad i = 1,\ldots,n, \tag{3.3}$$

$$\frac{\partial \mathcal{L}}{\partial \lambda_z} = 0, \quad z = 1,\ldots,m, \tag{3.4}$$

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[1] Minimization is an equivalent problem.

[2] For a more detailed description of this method see, e.g., Jehle (1991).

which is equivalent to

$$\pi_i = -\sum_{z=1}^{n} \lambda_z \frac{\partial g^z}{\partial x_i}, \quad i = 1, \ldots, n, \tag{3.5}$$

$$g^z = 0, \quad z = 1, \ldots, m, \tag{3.6}$$

where $\pi_i \equiv \frac{\partial y}{\partial x_i}$, $i = 1, \ldots, n$. The variable π_i is an **intensive variable**, i.e., a non-additive variable. If the function y and the constraints g^z are real valued and differentiable, if the number of constraints, m, is less than the number of variables, n, and if the gradient vectors of the constraint equations are linearly independent, the maximum exists. In this case, Lagrange's Method gives the first order **equilibrium conditions** [13], Eq. 3.5 and Eq. 3.6, which define the state of the system. The **differential form** of the fundamental equation is

$$dy = \sum_{i=1}^{n} \pi_i dx_i. \tag{3.7}$$

The constrained optimization problem in thermodynamics is the *maximization of entropy*, $S(U^1, U^2, V^1, V^2, N_1^1, N_1^2, \ldots, N_r^1, N_r^2)$, of a composite system, with subsystems 1 and 2 (see Appendix 3.13.1 for further details), with constant total internal energy, U, constant total volume, V, and constant total mole numbers for each chemical component, N_i, $i = 1, \ldots, r$, where N_i is the number of moles of the chemical compound i[3]. Thermodynamic intensive variables are:

$$\begin{aligned} 1/T^j &\equiv \partial S/\partial U^j, \\ P^j/T^j &\equiv \partial S/\partial V^j, \\ -\mu_i^j/T^j &\equiv \partial S/\partial N_i^j, \end{aligned} \tag{3.8}$$

with $j = 1, 2$ and $i = 1, \ldots, r$, where T^j is the temperature, P^j is the pressure and μ_i^j is the chemical potential of the i component of subsystem j. Temperature is defined positive by Nernst's postulate [4]. For the thermodynamic system, the equilibrium conditions (Eq. 3.5) are: $1/T^1 = 1/T^2 \equiv 1/T$, $P^1/T^1 = P^2/T^2 \equiv P/T$ and $\mu_i^1/T^1 = \mu_i^2/T^2 \equiv \mu_i/T$ with $i = 1, \ldots, r$. Thus, an isolated composite system with the above constraints increases its entropy towards the maximum value by turning into a system with a homogeneous temperature, homogeneous pressure and homogeneous chemical potentials for all compounds. The differential form of the fundamental equation is

$$dS = \sum_{j=1}^{2} \frac{1}{T^j} dU^j + \sum_{j=1}^{2} \frac{P^j}{T^j} dV^j - \sum_{j=1}^{2} \sum_{i=1}^{r} \frac{\mu_i^j}{T^j} dN_i^j. \tag{3.9}$$

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[3] It is considered that no chemical reactions occur.

The extremum principle, in consumer theory, is the *maximization of utility*, $U(x_1, \ldots, x_n)$, of a consumer at constant market prices, p_i, and constant endowment given by $w = p_1 x_1^0 + \ldots + p_n x_n^0$ where x_i, i = 1,..., n, are the available amounts of each good. The utility function, U, is the consumer's fundamental equation because it describes its behavior: when allowed to trade with the market, the consumer behaves in order to maximize his utility. The consumer intensive variables are the marginal utility of good i,

$$MU_i \equiv \partial U / \partial x_i. \tag{3.10}$$

Marginal utilities are defined positive by the assumption of monotonicity usually made on the utility function (Axiom 5, [13]): if a consumption bundle involves more of at least one good and no less of any other good, then it provides a higher utility than the original consumption bundle. This is equivalent to assuming that there are no 'bads', only goods [4]. The equilibrium conditions (Eq. 3.5) for the consumer are: $MU_1/p_1 = \ldots = MU_n/p_n$. Thus, a consumer whose constraints are that the endowment and the prices remain constant increases his utility towards the maximum value by exchanging with the market until the ratio of marginal utility to price is the same for all products. The differential form of the fundamental equation is

$$dU = MU_1 dx_1 + \ldots + MU_n dx_n. \tag{3.11}$$

3.3 Duality Formulation

A **duality formulation** of the fundamental equation is the inverse function $x_1 = x_1(y, x_2, \ldots, x_n)$. Its intensive variables are given by:

$$\begin{aligned} \frac{\partial x_1}{\partial y} &= \frac{1}{\pi_1} \\ \frac{\partial x_1}{\partial x_j} &= -\frac{\pi_j}{\pi_1}, \quad j = 2, \ldots, n. \end{aligned} \tag{3.12}$$

The duality formulation also has an extremum principle if y is a monotonically increasing function of x_1, i.e., $\pi_1 > 0$:

$$\begin{aligned} &\min_{y, x_2, \ldots, x_n} \quad x_1(y, x_2, \ldots, x_n) \quad s.t. \\ &g^z\left(y, x_2, \ldots, x_n, y^0, x_2^0, \ldots, x_n^0, k_1, \ldots, k_l\right) = 0, \\ &\qquad z = 1, \ldots, m. \end{aligned} \tag{3.13}$$

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[4] This is a simplification because 'bads' do exist, e.g., air pollution.

The proof by reduction to absurd is a generalization of theorem 4.3.2 given by Jehle [13]. If $y^* = \max y$ but $x_1^* \neq \min x_1$ then there exists at least $y^{*,a}(x_1^{*,a}, x_2, \ldots, x_n)$ $= y^*(x_1^*, x_2, \ldots, x_n)$ such that $x_1^{*,a} < x_1^*$. Since x_1 is increasing in y then $y^* > y^{*,a}$ which contradicts the initial assumption.

In the thermodynamic system, the duality is between entropy and energy. Entropy is a concave function and an increasing function of the internal energy, i.e., $\partial^2 S/\partial U^2 < 0$ and $\partial S/\partial U > 0$ which means that the internal energy is a convex function. Thus, the fundamental equation can also be written in the energy representation, $U(S^1, S^2, V^1, V^2, N_1^1, N_1^2, \ldots, N_r^1, N_r^2)$ (see Appendix 3.13.1 for further details); in this formulation the relevant extremum principle is the *Energy Minimum Principle*. In the energy representation, the intensive variables are straightforwardly the temperature, the (minus) pressure and the chemical potentials.

An intuitive explanation for the Energy Minimum Principle is the following: if the thermodynamic system is in equilibrium then its entropy is maximum, but if the energy is not in its minimum value then this quantity ‘in excess’ can be withdrawn from the system keeping the entropy constant. This quantity can then be returned to the system increasing the entropy because temperatures are positive. Thus, the initial state was not an equilibrium state because it was not at the maximum entropy [4].

In the consumer system, the duality is between utility and product demand. Utility is a concave function and an increasing function of the amount of product, i.e., $\partial^2 U/\partial x_i^2 < 0$ and $\partial U/\partial x_i > 0$ which means that the product demand function is a convex function. Thus, the fundamental equation can also be written in the product demand representation, $x_i(U, x_1, \ldots, x_{j\neq i}, \ldots, x_n)$. This equation represents the demand for product i as a function of utility and the amounts of the other products. In the product demand representation the extremum principle is the *Product Minimum Principle*.

An intuitive explanation for the Product Minimum Principle is the following: if the consumer system is in equilibrium then its utility is maximum, but if the consumption of product i is not in its minimum value then this quantity ‘in excess’ can be withdrawn from the system keeping the utility constant. This quantity could be later returned to the system increasing the utility because marginal utilities are positive. Thus, the initial state was not an equilibrium state because the consumer was not at the maximum utility.

The economic variables $x_1, \ldots, x_n$, in contrast to the thermodynamic variables, have a similar meaning, in the sense that, using prices, they can all be added. Therefore, the Product Minimum Principle can be applied for each product, implying that the feasible bundle is the one with the lowest amount of each product and the lowest cost. The explanation is that if the consumer did not choose the bundle with the lowest cost, he could trade it for a bundle with the same utility but a lower cost and use the remaining budget to buy goods and increase his utility. In consumer theory, this is known as (1) the duality between maximum utility and minimum expenditure, $E(x_1, \ldots, x_n) = \sum_{i=1}^{n} p_i x_i$ or (2) the equivalence between maximum utility and the cheapest bundle that provides that utility (axiom 5, [13]). While the maximum utility problem computes the maximum level of utility given a certain endowment, w, the minimum expenditure problem computes the minimum endowment required to reach a certain level of utility [18].

3.4 Reversible, Irreversible and Impossible Processes

The evolution of the system from the initial to the final state as described by Eq. 3.1, is triggered by a change in parameters; this is called a one step process. In a **reversible process**, the initial and final states have equal y. In an **irreversible process**, the final state has a higher value of y than the initial state. The amount of irreversibility (always positive) produced in an irreversible process can be measured by the increase in y. An **impossible process** is a process that will never occur because if it did the final state would have a lower value of of y.

Reversible processes in a thermodynamic system are processes that occur in an isolated system [5] at constant maximal entropy. An impossible process is a process that will never occur because if it did the maximum entropy of an isolated system would decrease. Irreversible processes in a thermodynamic system are processes that occur in an isolated system at increasing maximal entropy. The amount of irreversibility produced is equal to the variation in entropy between the initial state and the equilibrium state.

Reversible processes for the consumer are processes in which he trades at constant endowment with the market but does not increase his maximum utility. Impossible processes are trades that do not occur because the consumer with a constant endowment would decrease his maximum utility. Irreversible processes for the consumer are processes characterized by an increase in utility: if a consumer with constant endowment engages in a trade that increases his utility, he will not reverse the trade. The amount of irreversibility produced is equal to the amount of utility increase between the initial state and the equilibrium state.

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[5] An isolated thermodynamic system is a system with the set of constraints defined in Sec. 3.2.

3.5 Many-step Processes

The evaluation of the change in the equilibrium value of the potential function, y^*, in response to the change in its parameters is known as *comparative statics* analysis.

Given a change in parameters $dk_i, dk_j, \ldots$, the optimal values x_i^*, as a function of the parameters and of the initial conditions,

$$x_i^* = x_i^*(k_1, \ldots, k_l, x_1^0, \ldots, x_n^0), \tag{3.14}$$

are obtained from the equilibrium conditions, Eq. 3.5 and 3.6, and the optimal **value function** y^*,

$$y^* = y^*(k_1, \ldots, k_l, x_1^0, \ldots, x_n^0), \tag{3.15}$$

is obtained from the set of Eq. 3.14. Thus, Eq. 3.14 and 3.15 can be used to study a **many-step process** composed of many maximization steps where: (1) each maximization step is given by Eq. 3.1 and triggered by a change in one or more parameters and (2) the optimal value of x_i obtained at the end of each step is the initial value for the following step.

Not all trajectories described by Eq. 3.14 and 3.15 are processes because not all parameters are independent of each other. Suppose that $k_1(k_2, k_3)$; in this case, it is not possible to impose independently dk_1, dk_2 and dk_3.

Quasi-static Processes are processes characterized by infinitesimally close equilibrium points y^*; this requires infinitesimal changes in the parameters. Quasi-static processes are reversible, irreversible or impossible according to the criteria defined.

The effects of changes dk_i in the value function y^* are addressed by the **envelope theorem** summarized next (for more details consult [18]). Assuming that y^* is differentiable then at the equilibrium $x_1^*, \ldots, x_n^*$:

$$\frac{\partial y^*}{\partial k_i} = \frac{\partial y}{\partial k_i} - \sum_{z=1}^{m} \lambda_z \frac{\partial g^z}{\partial k_i}. \tag{3.16}$$

For the thermodynamic system, Eq. 3.14 is, e.g., $U_1^*(U, V, N_1, \ldots, N_r)$ while Eq. 3.15 is $S^*(U, V, N_1, \ldots, N_r)$.

The application of the envelope theorem to the maximization of entropy gives:

$$\begin{aligned} \frac{\partial S^*}{\partial U} &= -\lambda_1 = \frac{1}{T}, \\ \frac{\partial S^*}{\partial V} &= -\lambda_2 = \frac{P}{T}, \\ \frac{\partial S^*}{\partial N_i} &= -\lambda_j = -\frac{\mu_i}{T}, \quad j = 3, \ldots, r+2. \end{aligned} \tag{3.17}$$

The application of the envelope theorem to the minimization of energy gives:

$$\begin{aligned}\frac{\partial U^*}{\partial S} &= -\lambda_1 = && T, \\ \frac{\partial U^*}{\partial V} &= -\lambda_2 = && -P, \\ \frac{\partial U^*}{\partial N_i} &= -\lambda_j = && \mu_i, \quad j = 3, \ldots, r+2.\end{aligned} \tag{3.18}$$

For the consumer, Eq. 3.14 is the *Walrasian demand function* given by $x_i^*(w, p_1, \ldots, p_n)$ while Eq. 3.15 is the *indirect utility function*, $U^*(w, p_1, \ldots, p_n)$. For a given a set of prices and endowment, the Walrasian demand function specifies the amount of product x_i that maximizes utility while the indirect utility function specifies the maximum utility achievable.

The *Engel curve* is the Walrasian demand function with constant prices [18]. The Engel curve does not depict a process because endowment is a function of prices, $w(p_1, \ldots, p_n)$, i.e., it is not possible to change endowment while keeping all prices constant. It would only depict a process if at the end of each process the consumer either (1) had completely consumed all its goods and received a new amount of money equal to $w + dw$ or (2) exchanged all its goods for money and then received the extra endowment dw. These are not the conditions assumed for a many-step process.

The *offer curve* depicts the relation between price p_i and the optimal quantity of good i with all other prices and endowment constant, [18]. Like the Engel curve, the offer curve does not depict a process because $p_i(w, p_1, \ldots, p_{j,\forall j \neq i}, \ldots, p_n)$, i.e., it is not possible to change the price of good i while keeping all other prices and the endowment constant.

For the minimum expenditure representation, Eq. 3.14 is the *Hicksian demand function* given by $x_i^{h,*}(U, p_1, \ldots, p_n)$ while Eq. 3.15 is the expenditure function given by $w^*(U, p_1, \ldots, p_n)$. Maintaining a specified level of utility given a set of prices requires the amounts of products x_i, $i = 1, \ldots, n$, given by the Hicksian demand function and the endowment specified by the expenditure function.

The application of the envelope theorem for the maximization of utility gives

$$\begin{aligned}\frac{\partial U^*}{\partial p_i} &= -\lambda x_i^*, \\ \frac{\partial U^*}{\partial w} &= \lambda.\end{aligned} \tag{3.19}$$

Combining these results yields *Roy's Identity* [18]:

$$x_i^* = -\frac{\frac{\partial U^*}{\partial p_i}}{\frac{\partial U^*}{\partial w}}. \tag{3.20}$$

Roy's identity gives a method to obtain the Walrasian demand functions knowing the indirect utility functions. The intuition is the following: the higher the amount of x_i that a consumer needs to maximize his utility, the higher is the dependence of the maximum utility on p_i relative to its dependence on endowment. The application of the envelope theorem for the minimization of expenditure yields *Shepard's Lemma* [18]:

$$x_i^{h,*} = \frac{\partial w^*}{\partial p_i}. \tag{3.21}$$

Shephard's lemma gives a relationship between the Hicksian demand and the expenditure function. The intuition is the following: the higher the amount of x_i that a consumer needs to maintain his utility, the higher must be the expenditure increase with an increase in p_i to maintain the same utility.

3.6 Legendre Transforms

The **Legendre transform** is a mathematical technique by which one or more of the partial derivatives π_i replace one or more of the extensive variables x_i as independent variables. If the substitution of x_i by π_i is made for one variable, the Legendre transform is

$$\varphi_i(x_1, \dots, \pi_i, \dots, x_n) = y(x_1, \dots, x_n) - \pi_i x_i, \tag{3.22}$$

if it is is made for all variables, we have the complete Legendre transform

$$\varphi\left(\pi_1, \dots, \pi_i, \dots, \pi_n\right) = y\left(x_1, \dots, x_n\right) - \sum_{i=1}^{n} \pi_i x_i. \tag{3.23}$$

The meaning of the Legendre transform is easily grasped for two simplified cases: (1) the fundamental equation is a first order homogeneous function, i.e., the *Euler Equation*, $\pi_1 x_1 + \ldots + \pi_n x_n = y$, applies (see Appendix 3.13.4 for further details), implying that:

$$\varphi_i\left(x_1, \dots, \pi_i, \dots, x_n\right) = \sum_{j \neq i} \pi_j x_j, \tag{3.24}$$

(2) π_i is constant implying that the differential of the Legendre transform simplifies to: $d\varphi_i(x_1, \dots, \pi_i, \dots, x_n) = dy - \pi_i dx_i = \sum_{j \neq i} \pi_j dx_j$.

Suppose that an extremum principle applies to the initial function and to its Legendre transform. The Langrangean of the Legendre transform is

$$L(x_1, \dots, x_n, \lambda_1, \dots, \lambda_n) = \tag{3.25}$$

$$\overbrace{y(x_1,\ldots,x_w,\ldots,x_n)-\pi_w x_w}^{\varphi(x_1,\ldots,\pi_w,\ldots,x_n)}$$
$$+\sum_{z=1,m}\lambda'_z g'^z(x_1,\ldots,\pi_w,\ldots,x_n),$$

and the Lagrangean of function y is given by Eq. 3.2. The first order conditions to the optimization problems are respectively:

$$-\sum_{i=1,n}\lambda'_z\frac{\partial g'^z(x_1,\ldots,x_n)}{\partial x_{i\neq w}}=\frac{\partial\varphi(x_1,\ldots,\pi_w,\ldots,x_n)}{\partial x_{i\neq w}}=\pi'_i, \tag{3.26}$$

and Eq. 3.5. If π_w is constant, then $\pi_i = \pi'_i$ for all $i \neq w$ and Eq. 3.26 is equal to Eq. 3.5. Thus, whenever an extremum principle is imposed on the original function and π_w remains constant, an extremum principle is also imposed on the Legendre transform. Theorem 2.3.3 [13] determines the sufficient conditions for the constrained optimal point to be either a maximum or a minimum (see a more detailed discussion in sec. 3.9). According to this theorem the extremum is a constrained maximum if the principal minors of the Hessian matrix of the Lagrangean evaluated at the extremum alternate in sign beginning with positive (Appendix 3.13.2). The extremum is a constrained minimum if the principal minors of the Hessian matrix of the Lagrangean evaluated at the extremum are all negative. Whenever π_w is constant then (1) if the initial function is maximized, the same occurs with the Legendre transform and (2) if the initial function is minimized, the same occurs with the Legendre transform. This is because the Hessian matrix of the Lagrangian of the fundamental function is equal to the Hessian matrix of the Lagrangean of the Legendre transform.

In thermodynamics, intensive variables are constant when the system is no longer isolated but in contact with a reservoir that maintains, e.g., a constant temperature. The most common Legendre transforms in thermodynamics are (1) the *Helmholtz potential*, $F \equiv U - TS$; (2) the *Enthalpy*, $H \equiv U + PV$ and (3) the *Gibbs potential* $G \equiv U - TS + PV$ (for further details see Appendix 3.13.1). The extremum principles are: (1) the system reaches the minimum Helmholtz Energy subject to the reservoir temperature; (2) the system reaches the minimum Enthalpy subject to the reservoir pressure and (3) the system reaches the minimum Gibbs Energy subject to the reservoir pressure and temperature. The differential form of the Legendre transforms with constant intensive properties are:(1) $dF = dU - TdS$, (2) $dH = dU + PdV$, and (3) $dG = dU - TdS + PdV$.

For the consumer the Legendre transforms have an extremum principle when one or more of the marginal utilities are constant, i.e., the consumption of these goods is such that their marginal utilities are constant. For example: (1) Public Goods or non-excludable goods that have a null price and therefore null marginal utilities, i.e., these goods are consumed until the additional utility derived from their consumption is null and (2) rationed goods. These Legendre transforms have the following general form: $\Psi \equiv U - \sum\limits_{i=1,l} x_i MU_i$. The extremum principle is that the system reaches the maximum Ψ subject to constant marginal utilities for the products x_i, $i = 1, \ldots, l$. In this case, the differential form of the Legendre transforms is: $d\Psi = dU - \sum\limits_{i=1,l} MU_i dx_i = \sum\limits_{i=l+1,n} MU_i dx_i$. The economic intuition is that the consumer maximizes the utility obtained with the consumption of goods $i = l+1, \ldots, n$, because the amount of other goods is constrained in order to provide constant marginal utilities.

The complete Legendre transform $\Psi \equiv U - \sum\limits_{i=1,n} x_i MU_i$ can be written as the difference in the utility gain from consumption and a measure of the cost of consumption, $\Psi = U - \frac{MU_q}{p_q} \sum\limits_{i=1,n} x_i p_i$ where $\frac{MU_q}{p_q}$, is equal for all goods, in equilibrium. If marginal utilities are null then the complete Legendre transform is equal to the utility. Thus, the complete Legendre transform is a measure of the net benefits of consumption, i.e., *consumer's surplus* [38].

3.7 Elasticities

While the first derivatives of the fundamental equation are intensive variables, the second derivatives, i.e., elasticities, stand for important properties of the system. The non-dimensional **elasticities** have the general form

$$q^{ij}_{\Pi,X} = \frac{\pi_j}{x_i} \left(\frac{\partial x_i}{\partial \pi_j} \right)_{\Pi,X}, \tag{3.27}$$

where Π is the set of π_k variables kept constant (with $k \neq j$) and X is the set of x_z variables kept constant (with $z \neq i$) and the total number of variables kept constant is $n-1$. The absolute value of these non-dimensional elasticities has a straightforward interpretation: it is the ratio of the proportional change in x_i to the proportional change in π_j. These characteristics can be obtained empirically. Additionally,

$$\frac{1}{x_i} \frac{\partial (x_i \pi_i)}{\partial \pi_i} = 1 + \frac{\pi_i}{x_i} \frac{\partial x_i}{\partial \pi_i} = 1 + q^{ii}_{\Pi,X}, \tag{3.28}$$

which means that for $x_i > 0$ if (1) $q > -1$ then $\pi_i x_i$ increases with π_i while if (2) $q < -1$ then $\pi_i x_i$ decreases with π_i. If the fundamental equation is first order homogeneous then

$\pi_i x_i = \varphi(\pi_1, \ldots, x_i, \ldots, \pi_n)$ and the value of the non-dimensional elasticity determines the sign of the change in the potential given by the Legendre transform.

In thermodynamic systems, elasticities are descriptive of material properties. The most used elasticities are respectively the thermal expansion, the isothermal compressibility, the heat capacity at constant pressure, the adiabatic compressibility and the heat capacity at constant volume:

$$\begin{aligned} \alpha &\equiv \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_{P,N}, \\ \kappa_T &\equiv -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{T,N}, \\ c_P &\equiv T\left(\frac{\partial S}{\partial T}\right)_{P,N}, \\ \kappa_s &\equiv -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_{S,N}, \\ c_v &\equiv T\left(\frac{\partial S}{\partial T}\right)_{V,N}, \end{aligned} \tag{3.29}$$

(for further details see Appendix 3.13.1).

In thermodynamics non-dimensional elasticities are not used although they would be useful given Eq. 3.28. For example, consider a closed system with a movable and diathermic[6] wall in contact with a temperature reservoir. If the pressure of the reservoir is increased then: (1) the system is compressed by the reservoir until the pressures are equal and (2) a heat flow is established between the system and the reservoir to maintain the system at constant temperature. If the non-dimensional isothermal compressibility of the system $\kappa'_T = -\kappa_T P > -1$ then the change in internal energy associated with the increase in pressure will be positive, i.e., the change in the Legendre transform $d\phi(T, V, \mu) = d(-PV)$, while if $\kappa'_T < -1$, the change in internal energy associated with the increase in pressure will be negative. This is summarized for all thermodynamic non-dimensional elasticities in Tab. 3.1.

In economic systems, elasticities are descriptive of consumer characteristics. The non-dimensional elasticities used in consumer theory are called elasticities:

$$\varepsilon_{\{p_k, \forall k \neq i\}} \equiv \frac{p_i}{x_i}\left(\frac{\partial x_i}{\partial p_i}\right)_{\{p_k, \forall k \neq i\}}, \tag{3.30}$$

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[6] A diathermic wall allows for energy transfer in the form of heat between the system and the environment.

[7] Stability Conditions impose that $c'_P > 0$ (sec. 3.9).

[8] Stability Conditions impose that $c'_v > 0$ (sec. 3.9).

Elasticities	**Legendre transform behavior**
κ'_T	$\phi(T,V,\mu)$ increases with P at constant T if $\kappa'_T > -1$, remains constant if $\kappa'_T = -1$ and decreases otherwise.
κ'_s	$\phi(T,V,\mu)$ increases with P at constant S if $\kappa'_s > -1$, remains constant if $\kappa'_s = -1$ and decreases otherwise.
c'_P	$\phi(S,-P,\mu)$ increases with T at constant P if $c'_P > -1$ [7]
c'_v	$\phi(S,-P,\mu)$ increases with T at constant V if $c'_v > -1$ [8]

Table 3.1: The relation between Adimensional Thermodynamic Elasticities and the change in the potentials given by the Legendre transforms of the Energy Function.

$$\begin{aligned}
\varepsilon_{\{x_k,\forall k\neq j\}} &\equiv \frac{p_j}{x_j}\left(\frac{\partial x_j}{\partial p_j}\right)_{\{x_k,\forall k\neq j\}} \\
e_{\{p_k,\forall k\neq i\}} &\equiv \frac{p_i}{x_j}\left(\frac{\partial x_j}{\partial p_i}\right)_{\{p_k,\forall k\neq i\}}, \\
e_{\{x_k,\forall k\neq j\}} &\equiv \frac{p_i}{x_j}\left(\frac{\partial x_j}{\partial p_i}\right)_{\{x_k,\forall k\neq j\}}, \\
\mathfrak{e}_{\{p_k,\forall k\neq i\}} &\equiv \frac{w}{x_i}\left(\frac{\partial x_i}{\partial w}\right)_{\{p_k,\forall k\neq i\}}.
\end{aligned}$$

The $\varepsilon_{\{p_k,\forall k\neq i\}}$ is the adimensionalization of the inverse demand curve. It is called the own price elasticity of demand. It measures how responsive demand is to changes in price [38]. Products are classified as *Giffen Goods* if $\varepsilon_{\{p_k,\forall k\neq i\}} >0$. A product has an elastic demand if the absolute value of the own-price elasticity is higher than 1 and an inelastic demand otherwise. Eq. 3.28 says that if the demand of x_i is elastic then an increase in price will decrease the amount demanded so much that the revenue will decrease; if the demand is inelastic then an increase in price will not change demand very much and the overall revenue will increase. The $e_{\{p_k,\forall k\neq i\}}$ is called the cross-price elasticity of demand [13]. The $\varepsilon_{\{x_k,\forall k\neq j\}}$ and $e_{\{x_k,\forall k\neq j\}}$ are also prices elasticities but with the amounts of other products kept constant. The $\mathfrak{e}_{\{p_k,\forall k\neq i\}}$ is the adimensionalization of the inverse income curve. It is called the income elasticity of demand. It measures how responsive demand is to some change in income [38]. Products are classified according to their income elasticity: *normal goods* ($\mathfrak{e}_{\{p_k,\forall k\neq i\}} >0$) and *inferior goods* ($\mathfrak{e}_{\{p_k,\forall k\neq i\}} <0$). Normal goods can be either *necessary goods* ($\mathfrak{e}_{\{p_k,\forall k\neq i\}} < 1$) or *luxury goods* ($\mathfrak{e}_{\{p_k,\forall k\neq i\}} >1$). In the consumer elasticities, prices are used instead of marginal utilities, because in equilibrium marginal utilities are proportional to prices.

y	$\left(\frac{\partial \pi_i}{\partial x_j}\right)_{\{x_k,\forall k\neq j\}}$	=	$\left(\frac{\partial \pi_j}{\partial x_i}\right)_{\{x_z,\forall z\neq i\}}$
φ_i	$\left(\frac{\partial \pi_l}{\partial x_j}\right)_{\pi_i,\{x_k,\forall k\neq i,j\}}$	=	$\left(\frac{\partial \pi_j}{\partial x_l}\right)_{\pi_i,\{x_z,\forall z\neq i,l\}}$
$\varphi_{i,g}$	$\left(\frac{\partial \pi_l}{\partial x_j}\right)_{\pi_i,\pi_g,\{x_k,\forall k\neq i,j,g\}}$	=	$\left(\frac{\partial \pi_j}{\partial x_l}\right)_{\pi_i,\pi_g,\{x_z,\forall z\neq i,l,g\}}$
φ_i	$\left(\frac{\partial \pi_k}{\partial \pi_i}\right)_{\{x_j,\forall j\neq i\}}$	=	$-\left(\frac{\partial x_i}{\partial x_k}\right)_{\pi_i,\{x_j,\forall j\neq i,k\}}$
$\varphi_{i,g}$	$\left(\frac{\partial \pi_k}{\partial \pi_i}\right)_{\pi_g,\{x_j,\forall j\neq i,g\}}$	=	$-\left(\frac{\partial x_i}{\partial x_k}\right)_{\pi_i,\pi_g,\{x_j,\forall j\neq i,k,g\}}$
$\varphi_{i,g}$	$\left(\frac{\partial x_i}{\partial \pi_g}\right)_{\pi_i,\{x_j,\forall j\neq i,g\}}$	=	$\left(\frac{\partial x_g}{\partial \pi_i}\right)_{\pi_g,\{x_j,\forall j\neq i,g\}}$
φ	$\left(\frac{\partial x_i}{\partial \pi_g}\right)_{\{\pi_j,\forall j\neq g\}}$	=	$\left(\frac{\partial x_g}{\partial \pi_i}\right)_{\{\pi_j,\forall j\neq i\}}$

Table 3.2: Maxwell Relations obtained from $y = y(x_1, \ldots, x_n)$ and its Legendre transforms $\varphi_i = \varphi_i(x_1, \ldots, \pi_i, \ldots, x_n)$, $\varphi_{i,g} = \varphi_{i,g}(x_1, \ldots, \pi_i, \pi_g, \ldots, x_n)$ and $\varphi = \varphi(\pi_1, \ldots, \pi_n)$.

3.8 Maxwell Relations

The **Maxwell Relations** result from the equality of mixed partial derivatives valid for scalar functions whose second derivatives exist and are continuous (Young's Theorem). The equality between the mixed partial derivatives of the fundamental equation $y = y(x_1, \ldots, x_n)$ implies that:

$$\left(\frac{\partial \pi_i}{\partial x_j}\right)_{x_{k\neq j}} = \left(\frac{\partial \pi_j}{\partial x_i}\right)_{x_{k\neq i}}. \tag{3.31}$$

The equality between the mixed partial derivatives is also applicable to the other formulations of the fundamental equation, i.e., the Duality Formulation and the Legendre transforms. The Maxwell Relations for the Legendre transforms are given in Tab. 3.2.

Maxwell relations are important because they make explicit that not all second mixed derivatives are independent. In fact, all second derivatives can be written as a function of a small set of independent variables. The relations between the elasticities,

$$q^{kk}_{\{\pi_i,\forall i\neq k\}} = q^{kk}_{x_j,\{\pi_i,\forall i\neq k,j\}} + \frac{\left(q^{jk}_{\{\pi_i,\forall i\neq k\}}\right)^2}{q^{jj}_{\{\pi_i,\forall i\neq j\}}}\frac{\pi_j x_j}{\pi_k x_k}, \tag{3.32}$$

$$q^{kk}_{x_j,\{\pi_i,\forall i\neq k,j\}} = q^{kk}_{x_j,x_z,\{\pi_i,\forall i\neq k,j,z\}} + \frac{\left(q^{zk}_{x_j,\{\pi_i,\forall i\neq k,j\}}\right)^2}{q^{zz}_{x_j\{\pi_i,\forall i\neq j,z\}}}\frac{\pi_z x_z}{\pi_k x_k}, \tag{3.33}$$

$$\ldots$$

$U(S,V,N)$	$\left(\frac{\partial T}{\partial V}\right)_{S,N} = -\left(\frac{\partial P}{\partial S}\right)_{V,N}$	$\left(\frac{\partial T}{\partial N}\right)_{S,V} = \left(\frac{\partial \mu}{\partial S}\right)_{V,N}$	$\left(\frac{\partial P}{\partial N}\right)_{S,V} = -\left(\frac{\partial \mu}{\partial V}\right)_{S,N}$
$F(T,V,N)$	$\left(\frac{\partial S}{\partial V}\right)_{T,N} = \left(\frac{\partial P}{\partial T}\right)_{V,N}$	$\left(\frac{\partial S}{\partial N}\right)_{T,V} = -\left(\frac{\partial \mu}{\partial T}\right)_{V,N}$	$\left(\frac{\partial P}{\partial N}\right)_{T,V} = -\left(\frac{\partial \mu}{\partial V}\right)_{T,N}$
$H(S,P,N)$	$\left(\frac{\partial T}{\partial P}\right)_{S,N} = \left(\frac{\partial V}{\partial S}\right)_{P,N}$	$\left(\frac{\partial T}{\partial N}\right)_{S,P} = \left(\frac{\partial \mu}{\partial S}\right)_{P,N}$	$\left(\frac{\partial V}{\partial N}\right)_{S,P} = \left(\frac{\partial \mu}{\partial P}\right)_{S,N}$
$G(T,P,N)$	$\left(\frac{\partial S}{\partial P}\right)_{T,N} = -\left(\frac{\partial V}{\partial T}\right)_{P,N}$	$\left(\frac{\partial S}{\partial N}\right)_{T,P} = -\left(\frac{\partial \mu}{\partial T}\right)_{P,N}$	$\left(\frac{\partial V}{\partial N}\right)_{T,P} = \left(\frac{\partial \mu}{\partial P}\right)_{T,N}$

Table 3.3: Thermodynamic Maxwell Relations obtained from U, F, H and G.

$$q^{kk}_{\pi_l,\{x_i,\forall i\neq l,k\}} = q^{kk}_{\{x_i,\forall i\neq k\}} + \frac{\left(q^{lk}_{\pi_l,\{x_i,\forall i\neq l,k\}}\right)^2}{q^{ll}_{\pi_k,\{x_i,\forall i\neq l,k\}}}\frac{\pi_l x_l}{\pi_k x_k}, \tag{3.34}$$

are obtained using the Maxwell relations (see Appendix 3.13.3 for further details). The relation between $q^{kk}_{\pi_{i\neq k}}$ and $q^{kk}_{x_{i\neq k}}$ (see also Appendix 3.13.3 for further details) is:

$$\begin{aligned} q^{kk}_{\{\pi_i,\forall i\neq k\}} &= q^{kk}_{\{x_i,\forall i\neq k\}} + \\ \sum_{j\neq k}\frac{x_j\pi_j}{x_k\pi_k}&\frac{q^{jk}_{\{\pi_i,\forall i\neq k\}}q^{jk}_{\pi_j,\{x_i,\forall i\neq j,k\}}}{q^{jj}_{\pi_k,\{x_i,\forall i\neq j,k\}}}. \end{aligned} \tag{3.35}$$

The Maxwell relations that result from the Energy representation of the fundamental equation and its Legendre transforms are given in Tab. 3.3 and the relations between the thermodynamic elasticities for constant mole numbers are presented next.

The relation between the specific heat at constant pressure and the specific heat at constant volume,

$$c_P = c_v + \frac{Tv\alpha^2}{\kappa_T}, \tag{3.36}$$

is obtained using Eq. 3.33 and the relation between the adiabatic compressibility and compressibility at constant temperature,

$$\kappa_T = \kappa_s + \frac{Tv\alpha^2}{c_P}, \tag{3.37}$$

is obtained using Eq. 3.33 and the Maxwell Relation $\left(\frac{\partial S}{\partial P}\right)_{T,N} = -\left(\frac{\partial V}{\partial T}\right)_{P,N}$. Eq. 3.36 and 3.37 imply that only three of five coefficients defined by Eq. 3.29 are independent. The relation between specific heats and compressibilities is

$$\frac{c_P}{c_v} = \frac{\kappa_T}{\kappa_s}. \tag{3.38}$$

The Maxwell relations that result from the Utility function and its Legendre transforms are given in Tab. 3.4 and the relations between the economic elasticities for two products are summarized next.

$U(x_1, \ldots, x_n)$	$\left(\frac{\partial p_i}{\partial x_j}\right)_{\{x_k, \forall k \neq j\}}$	=	$\left(\frac{\partial p_j}{\partial x_i}\right)_{\{x_k, \forall k \neq i\}}$
$\varphi_i\left(x_1, \ldots, p_i, \ldots, x_n\right)$	$-\left(\frac{\partial p_j}{\partial p_i}\right)_{\{x_k, \forall k \neq i\}}$	=	$\left(\frac{\partial x_i}{\partial x_j}\right)_{p_i, \{x_k, \forall k \neq i,j\}}$
$\varphi_i\left(x_1, \ldots, p_i, \ldots, x_n\right)$	$\left(\frac{\partial p_j}{\partial x_k}\right)_{p_i, \{x_l, \forall l \neq i,k\}}$	=	$\left(\frac{\partial p_k}{\partial x_j}\right)_{p_i, \{x_l, \forall l \neq i,j\}}$
$\varphi\left(p_1, \ldots, p_i, \ldots, p_m\right)$	$\left(\frac{\partial p_j}{\partial x_i}\right)_{\{p_k, \forall k \neq j\}}$	=	$\left(\frac{\partial p_i}{\partial x_j}\right)_{\{p_k, \forall k \neq i\}}$

Table 3.4: Economic Maxwell Relations obtained from U, φ_i and φ.

The relation between the own price elasticity of demand at constant prices and the own price elasticity of demand at constant amounts for product 2,

$$\varepsilon_{p_2} = \varepsilon_{x_2} + e_{p_2}^2 \frac{1}{\varepsilon_{p_1}} \frac{p_2 x_2}{p_1 x_1}, \tag{3.39}$$

is obtained using Eq. 3.33 and for product 1,

$$\varepsilon_{p_1} = \varepsilon_{x_1} + e_{p_2}^2 \frac{1}{\varepsilon_{p_2}} \frac{p_2 x_2}{p_1 x_1}, \tag{3.40}$$

is obtained using Eq. 3.33 and the Maxwell relation $\left(\frac{\partial x_1}{\partial p_2}\right)_{p_1,N} = \left(\frac{\partial x_2}{\partial p_1}\right)_{p_2}$. Eq. 3.39 and 3.40 imply that only three of the elasticities defined by Eq. 3.30 are independent. The relation between the own price elasticities at constant prices and at constant amounts is

$$\frac{\varepsilon_{p_1}}{\varepsilon_{p_2}} = \frac{\varepsilon_{x_1}}{\varepsilon_{x_2}}. \tag{3.41}$$

3.9 Stability Conditions and the Le Chatelier Principle

The **stability of the equilibrium state** of a function y depends on the sign of d^2y. If the equilibrium is a maximum, the function is stable if it is strictly concave, i.e., $d^2y < 0$; if the equilibrium is a minimum, the function is stable if it is strictly convex, i.e., $d^2y > 0$. The sufficient condition for the twice continuously differentiable real-valued function y on a set C to be (1) strictly convex is that its Hessian matrix is positive definite, i.e., all sub matrices of the Hessian matrix defined by the first k rows and k columns have positive determinants and to be (2) strictly concave is that its Hessian matrix is negative definite, i.e., the determinants of the Hessian matrix are negative if k is odd and positive if k is even [22]. These necessary and sufficient conditions impose certain constraints on the signs of the elasticities (second derivatives).

Function $y(x_1, \ldots, x_n)$ is strictly concave if $(\partial \pi_i)/(\partial x_i)_{\{x_k, \forall k \neq i\}} < 0$, i.e., $q^{kk}_{\{x_k, \forall k \neq i\}} < 0$ if $\pi_i > 0$ and $x_i > 0$. The Legendre transforms of the concave function y are convex with respect to its intensive variables (a proof is presented in sec. 3.6), i.e., its second derivatives are positive

$$\begin{aligned}\frac{\partial^2\varphi(x_1,\ldots,x_l,\pi_{l+1},\ldots,\pi_n)}{\partial\pi_{l+1}^2} &= \\ -\frac{\partial x_{l+1}(x_1,\ldots,x_l,\pi_{l+1},\ldots,\pi_n)}{\partial\pi_{l+1}} &= \\ -\frac{x_{l+1}}{\pi_{l+1}}q_{\Pi,X}^{l+1,l+1} &> 0,\end{aligned} \tag{3.42}$$

with $\Pi = \{\pi_j, j = l+1,\ldots,n\}$ and $X = \{x_i, i = 1,\ldots,l\}$. Thus, the elasticity $q_{\Pi,X}^{l+1,l+1}$ in Eq. 3.42 is negative if $\pi_i > 0$ and $x_i > 0$. Additionally, Eq. 3.32 to Eq. 3.34 imply **the Generalized Le Chatelier Principle**: $0 > q^{kk}_{\{x_i,\forall i\neq k\}} > \ldots > q^{kk}_{x_j,\{\pi_i,\forall i\neq k,j\}} > q^{kk}_{\{\pi_i,\forall i\neq k\}}$.

The Generalized Le Chatelier Principle relations describe the behavior of a stable system displaced from equilibrium by a change in its extensive variable dx_k: (1) its conjugate intensive variable will change by $d\pi_k$ and (2) the absolute value of $d\pi_k$ increases with the number of extensive variables kept constant.

The entropy is strictly concave if $(\partial^2 S/\partial U^2) < 0$, i.e., $c_v > 0$. The Gibbs Energy is strictly concave on its intensive independent variables T and P, if $(\partial^2 G/\partial T^2) < 0$, i.e., $c_P > 0$, and that $(\partial^2 G/\partial P^2) < 0$, i.e., $\kappa_T > 0$. These constraints on c_v, c_P and κ_T together with Eq. 3.38 imply that $\kappa_s > 0$. Additionally, Eq. 3.36 and Eq. 3.37 imply that $c_P > c_v$ and $\kappa_T > \kappa_s$.

The conditions $(\partial^2 S/\partial U^2) < 0$ and $(\partial^2 S/\partial V^2) < 0$ imply that: (1) the amount of entropy increase that results from an unit increase in internal energy at constant volume (due to a heat flow) decreases with the internal energy of the system and (2) the amount of entropy increase that results from an unit increase of volume at constant internal energy (due to both heat and work flows) decreases with the volume of the system.

Conditions $c_P > c_v > 0$ and $\kappa_T > \kappa_s > 0$ embody the Generalized Le Chatelier Principle for thermodynamic systems: the absolute change in temperature triggered by a change in entropy is higher for a system at constant volume than for a system at constant pressure and the absolute change in pressure triggered by a change in volume is higher for a system at constant entropy than for a system at constant pressure. As an example, we can think of a diathermic cylinder fitted with a piston that is in contact with a temperature reservoir. Suppose that the piston is pulled and an increase in volume occurs. The system will decrease its pressure ($\kappa_T > 0$), but this decrease will be smaller ($\kappa_T > \kappa_s > 0$) than at constant entropy, because the system receives a flow of heat from the temperature

Thermodynamic Constraints	**Economic Constraints**
$c_P > c_v > 0$	$0 > \varepsilon_{\{x_k,\forall k\neq i\}} > \varepsilon_{\{p_k,\forall k\neq i\}}$
$\kappa_T > \kappa_s > 0$	

Table 3.5: Constraints on the thermodynamic and economic elasticities imposed by stability.

reservoir.

The utility is strictly concave if $(\partial^2 U/\partial x_i^2) < 0$, i.e., $\varepsilon_{\{x_k,\forall k\neq i\}} < 0$. The Economic Potential Ψ is strictly convex on its intensive variables MU_i if $\varepsilon_{\{p_k,\forall k\neq i\}} < 0$ and, Eq. 3.39 and Eq. 3.40 imply that $\varepsilon_{\{x_k,\forall k\neq i\}} > \varepsilon_{\{p_k,\forall k\neq i\}}$ (assuming that prices and amounts are positive). These stability results imply that Giffen goods do not exist if the equilibrium state is stable[9].

The condition $(\partial^2 U/\partial x_i^2) < 0$ corresponds to the ‘Law’ of Diminishing Marginal Utility: the utility gained from an extra increase of one unit of product x_i decreases with the amount of x_i already owned.

Conditions $0 > \varepsilon_{\{x_k,\forall k\neq i\}} > \varepsilon_{\{p_k,\forall k\neq i\}}$ embody the Generalized Le Chatelier Principle for the consumer: the absolute change in demand triggered by a change in price is higher for constant product amounts than for constant prices. As an example, we can think of a consumer in contact with a market that has only two goods. If the price of product p_1 decreases the consumer buys an additional amount of good x_1 ($\varepsilon_{p_2} < 0$). The amount of x_1 traded is smaller if the consumer can also trade product 2 with the market ($0 > \varepsilon_{x_2} > \varepsilon_{p_2}$).

Tab. 3.5 summarizes the constraints imposed by stability on the thermodynamic and economic elasticities.

3.10 Equations of State and Integrability

Equations of state are equations that establish a relation in equilibrium between one intensive variable and the independent extensive variables. They have the following functional form

$$\pi_i = \pi_i\left(x_1, x_2, \ldots, x_n\right).$$

The knowledge of all equations of state is equivalent to the knowledge of the fundamental equation under certain conditions. This is known as the **integrability problem** and it can be summarized as follows: ‘When is it possible to build a fundamental function using

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[9] Note that this would not occur if only quasi-concavity of the utility function was required (remark pointed out by one of the reviewers).

the equations of state?'. First, mathematical integrability implies that the fundamental equation must satisfy the Maxwell relations. Second, the optimization behavior embedded in the fundamental equation implies that the equations of state do not contradict that the behavior is indeed optimized, i.e., the Generalized Le Chatelier Principle is verified. These two conditions are equivalent to imposing that the Hessian matrix of the fundamental function is (1) symmetric and (2) negative semidefinite. If the fundamental equation represents an order relation [10] then these two conditions are met (for further details see Candeal et al. [6]).

In the thermodynamic system, the equations of state, derived from the fundamental equation written in the energy representation, are: $T = T(S, V, N_1, \ldots, N_r)$, $P = P(S, V, N_1, \ldots, N_r)$ and $\mu_j = \mu_j(S, V, N_1, \ldots, N_r)$ with $j = 1, \ldots, r$ (see Appendix 3.13.1 for further details). These equations can be computed based on observed behavior. The energy fundamental equation can be built knowing all the equations of state by using Eq. 3.18. We can identify the first condition of integrability in thermodynamics as the Maxwell relations and the second as the constraints imposed on the thermodynamic coefficients by the Generalized Le Chatelier Principle. In thermodynamics, the entropy represents a preference relation imposed by the second law (for further details see Cooper [7]); thus, it is always possible to obtain an entropy function from the equations of state.

In the consumer, the equations of state, derived from the fundamental equation written in the expenditure representation, are: $p_j = p_j(x_1, \ldots, x_n)$. These equations can be computed based on observed behavior. The expenditure function can be built knowing all the Walrasian demand functions (obtained from the equations of state) by using Eq. 3.20. The first condition of integrability is known in economics as *Antonelli's integrability condition* and the second condition, i.e., the constraints imposed on economic elasticities, is known as *'economic integrability'* [17]. In the consumer the utility represents a preference relation if and only if the consumer is rational; thus, it might not be possible to obtain a utility function from the equations of state.

3.11 First Order Phase Transitions

Phase transitions occur where the fundamental equation is unstable (at least one of the stability criteria is violated). In Fig.3.1, the fundamental equation is unstable where

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[10] A function f represents a preference relation $\preceq$ if: $x \preceq y \Leftrightarrow f(x) \leq f(y)$.

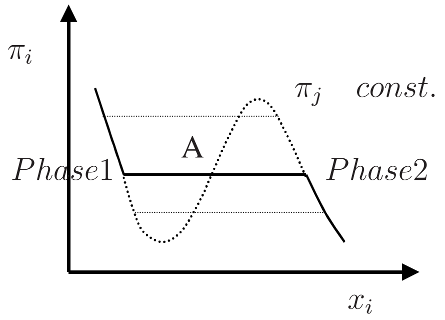

Figure 3.1: First Order Phase Transition.

$q^{ii}_{\{\pi_j,\forall j\neq i\}} > 0$, assuming that intensive and extensive variables are positive. In this case, the fundamental equation is no longer valid, i.e., the system is not characterized by the equilibrium conditions. However, the system can be decomposed into *phases*, i.e, subsystems in equilibrium.

The two states [11] between which a first order transition occurs are distinct and are characterized (1) by being in equilibrium with each other, i.e., by having equal intensive variables [14],

$$\pi^1_j = \pi^2_j, \qquad j = 1, \ldots, n, \tag{3.43}$$

where π^k_j is the intensive variable π_j in phase k, $k = 1, 2$ and (2) by having at least one extensive variable that is different $x^1_j \neq x^2_j$ where x^k_j is the extensive variable x_j in phase k. Conditions (1) and (2) imply that (3) $q^{jj}_{\{\pi_i,\forall i\neq j\}} = \infty$.

The number of intensive variables with an independent variation $d\pi_i$ in a system is called the number of degrees of freedom. If the system is homogeneous first order then the **Gibbs-Duhem Equation**,

$$0 = x_1 d\pi_1 + \ldots + x_n d\pi_n, \tag{3.44}$$

applies (see Appendix 3.13.4 for further details) and the number of degrees of freedom decreases to $n-1$. Otherwise, it has n degrees of freedom.

In a system whose y is homogeneous first order, in a phase transition, the **Gibbs-Duhem Equation**,

$$0 = x^k_1 d\pi_1 + \ldots + x^k_n d\pi_n, \tag{3.45}$$

applies to each phase k (see Appendix 3.13.4 for further details) and the number of degrees of freedom decreases to $f = n - 2$ because (1) the change in the intensive variables $d\pi_j$ and $d\pi_g$ can be written as a function of the other intensive variables (eq. 3.45) and (2)

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[11] More than two states are possible but will not be considered in this chapter.

Eq. 3.43 applies. This is the **Generalized Gibbs phase rule**. If y is not homogeneous first order then the number of degrees of freedom in phase transition is n.

The relation between the intensive variables $\pi_p \equiv \pi_p^1 = \pi_p^2$ and $\pi_g \equiv \pi_g^1 = \pi_g^2$ in equilibrium can be computed with the **Generalized Clapeyron Equation**:

$$\left(\frac{\partial \pi_p}{\partial \pi_g}\right)_{\{\pi_i^1-\pi_i^2,\forall i\neq p,g\}} = -\frac{\left(\frac{\partial\left(\pi_k^1-\pi_k^2\right)}{\partial \pi_g}\right)_{\{\pi_i^1-\pi_i^2,\forall i\neq k,g\}}}{\left(\frac{\partial\left(\pi_k^1-\pi_k^2\right)}{\partial \pi_p}\right)_{\{\pi_i^1-\pi_i^2,\forall i\neq k,p\}}} =$$

$$-\frac{\left(\frac{\partial \pi_k^1}{\partial \pi_g}\right)_{\{\pi_i^1-\pi_i^2,\forall i\neq k,g\}} - \left(\frac{\partial \pi_k^2}{\partial \pi_g}\right)_{\{\pi_i^1-\pi_i^2,\forall i\neq k,g\}}}{\left(\frac{\partial \pi_k^1}{\partial \pi_p}\right)_{\{\pi_i^1-\pi_i^2,\forall i\neq k,p\}} - \left(\frac{\partial \pi_k^2}{\partial \pi_p}\right)_{\{\pi_i^1-\pi_i^2,\forall i\neq k,p\}}}. \tag{3.46}$$

where $\pi_i^1 - \pi_i^2$ is constant and equal to zero (Eq. 3.43). If the potential y is a first order homogeneous function then Eq. 3.46 simplifies to

$$\left(\frac{\partial \pi_p}{\partial \pi_g}\right)_{\{\pi_i^1-\pi_i^2,\forall i\neq p,g\}} = -\frac{\frac{x_g^1}{x_k^1} - \frac{x_g^2}{x_k^2}}{\frac{x_p^1}{x_k^1} - \frac{x_p^2}{x_k^2}}, \tag{3.47}$$

by computing the partial derivatives using the Gibbs-Duhem Equation (Eq. 3.45) for each phase.

The system goes through a heterogeneous state where both phases coexist, with a fraction of the system in one phase and the remainder in the other. The intensive variables π_i that characterize the line that links the two phases (line A in Fig. 3.1) are such that:$\sum_{i\neq j} \int_{\pi_i^1}^{\pi_i^2} (x_i^1 - x_i^2) d\pi_i = 0$; this is the **Maxwell construction** proved next. Each point in a vertical line in Fig. 3.1 has a different π_i for $i \neq j$; therefore, vertical lines have a variable value of the Legendre transform $\varphi(\pi_1, \ldots, \pi_n)$. The horizontal line or π_i that correspond to the phase transition are such that the Legendre transform is at its maximum:

$$d\varphi = \sum_{i\neq j} x_i d\pi_i = 0. \tag{3.48}$$

By integrating Eq. 3.48 we obtain the Maxwell construction. Its geometrical meaning is best understood for the case where all intensive variables are kept constant with the exception of π_k: $\int_{\pi_k^1}^{\pi_k^2} x_k d\pi_k = 0$, i.e., the area below the dashed line must be equal to the area above. However, if the function y is homogeneous first order then the Legendre transform $\varphi(\pi_1, \ldots, \pi_n)$ is always null because Eq. 3.45 applies. In this case, the adequate

Legendre transform has one extensive variable, $\varphi(x_1, \pi_2, \ldots, \pi_n)$. Also, the horizontal line or the π_i that corresponds to the phase transition is such that the Legendre transform is at its maximum. With x_1 constant:

$$d\varphi = \sum_{i \neq 1,j} x_i d\pi_i = 0. \tag{3.49}$$

Also for systems where x_1 is constant and all intensive variables with the exception of π_k are also kept constant: $\int\limits_{\pi_k^1}^{\pi_k^2} x_k d\pi_k = 0$.

The system moves from one phase to the other by exchanging extensive variables with the exterior, i.e., **flows**, subject to the constraints imposed:

$$g^z = 0, \quad z = 1, \ldots, m. \tag{3.50}$$

The amount of an extensive variable, X, is computed with

$$X = X^1 + X^2 \equiv \alpha X + (1 - \alpha)X,$$

where X^k is the amount of X in phase $k = 1, 2$ and α is the fraction of X in phase 1. The amount of other extensive variables x_z^k in each phase k is

$$x_z^1 = X\alpha\mathcal{X}_z^1,$$
$$x_z^2 = X(1-\alpha)\mathcal{X}_z^2.$$

where $\mathcal{X}_z^k \equiv \frac{x_z^k}{X^k}$ are the specific extensive variables. Thus the amount of x_z is

$$x_z = x_z^1 + x_z^2 = X\alpha\mathcal{X}_z^1 + X(1-\alpha)\mathcal{X}_z^2. \tag{3.51}$$

This is the **Generalized Lever Rule**, i.e., the set of variables x_z, $z = 1, \ldots, n$ is a linear combination of the sets of specific variables $\mathcal{X}_z^k$, $k = 1, 2$.

The set of independent intensive variables completely specify the set of specific variables $\mathcal{X}_z^k$. With the set of specific variables $\mathcal{X}_z^k$ for $z = 1, \ldots, n$ and $k = 1, 2$, the set of Eq. 3.51 for $z = 1, \ldots, n$, the constraints imposed by Eq. 3.50, X and α it is possible to compute $x_z, \quad z = 1, \ldots, n$.

In a thermodynamic system, a phase transition occurs where the entropy fundamental equation is unstable, i.e., it is no longer concave. Fig. 3.2 shows where the stability criteria are violated: where the compressibility at constant temperature, κ_T, becomes negative. In this case, the system is no longer homogeneous but two different phases coexist. The two

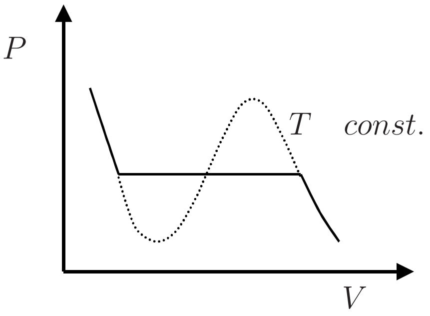

Figure 3.2: First Order Phase Transition in Thermodynamics.

phases are characterized by: (1) equal temperature, pressure and chemical potential for each chemical species and (2) different volumes, number of moles and internal energy. These conditions imply that $c_P = \infty, \alpha = \infty, \kappa_T = \infty$.

The number of independent intensive variables, given by the Gibbs phase rule, for thermodynamics, is $r = (r + 2) - 2$ where r is the number of different chemical species and $r+2$ is the number of extensive variables. For systems with constant number of moles, constant temperature and constant chemical potentials for all species, the horizontal line of the phase transition is such that: $\int\limits_{P^1}^{P^2} VdP = 0$ (Fig. 3.2).

In the thermodynamic phase transition, the change in pressure with temperature given by the Clapeyron Equation (Eq. 3.47) is

$$\left(\frac{\partial P}{\partial T}\right)_{\{\mu^1=\mu^2\}} = \frac{\frac{S^1}{N^1} - \frac{S^2}{N^2}}{\frac{V^1}{N^1} - \frac{V^2}{N^2}} = \frac{\Delta s}{\Delta v}, \tag{3.52}$$

obtained for a system with one chemical component using Eq. 3.47 with $\pi_p = -P$ and $\pi_g = T$ and where Δs and Δv are the changes in specific entropy, $s \equiv S/N$, and specific volume, $v \equiv V/N$, between the two phases. The other relations that can be obtained are:

$$\left(\frac{\partial \mu}{\partial T}\right)_{\{P^1=P^2\}} = -\frac{\frac{S^1}{V^1} - \frac{S^2}{V^2}}{\frac{N^1}{V^1} - \frac{N^2}{V^2}} = -\frac{s^1 v^2 - s^2 v^1}{\Delta v}, \tag{3.53}$$

and

$$\left(\frac{\partial \mu}{\partial P}\right)_{\{T^1=T^2\}} = \frac{\frac{V^1}{S^1} - \frac{V^2}{S^2}}{\frac{N^1}{S^1} - \frac{N^2}{S^2}} = \frac{v^1 s^2 - v^2 s^1}{\Delta s}. \tag{3.54}$$

In a thermodynamic system, the phase transition occurs as the system exchanges energy and/or volume, in the form of heat and/or work with the environment, i.e., U and/or V change during the phase transition, at constant total number of moles

$$N \equiv N^1 + N^2 = \alpha N + (1 - \alpha)N, \tag{3.55}$$

where α is the fraction of N in phase 1. The aggregate amounts of volume and internal energy are given by the *Lever Rule*: $V = V^1 + V^2 = \alpha N v^1 + (1-\alpha) N v^2$ and $U = U^1 + U^2 = \alpha N u^1 + (1-\alpha) N u^2$, where $v^k \equiv V^k/N^k$ is the specific volume and $u^k \equiv U^k/N^k$ is the specific energy in phase k.

Phase transitions in consumer theory occur where the utility function is unstable (no longer concave) or the expenditure function is unstable (no longer convex). Fig. 3.3 shows where the stability criteria are violated: the own price elasticity of demand, ε_{p_k}, becomes positive. In this case, the consumer has two different stable consumption bundles. The two consumption bundles are characterized by: (1) equal MU_i and (2) different values of the variables x_i. These conditions imply that $\varepsilon_{\{p_k, \forall k \neq i\}} = \infty$, $e_{\{p_k, \forall k \neq i\}} = \infty$, $\mathfrak{e}_{\{p_k, \forall k \neq i\}} = \infty$.

The number of independent intensive variables, given by the Gibbs phase rule, for the consumer, is n and decreases to $n-2$ is the utility is a first order homogeneous function. For consumers in a market with constant prices for all products except product k, the horizontal line of the phase transition is such that: $\int\limits_{p_k^1}^{p_k^2} x_k dp = 0$.

In the consumer phase transition, the change in price of good i with price of good j, is

$$\left(\frac{\partial p_i}{\partial p_j}\right)_{\{p_z^1 = p_z^2, \forall z \neq i,j\}} = -\frac{\left(\frac{\partial p_k^1}{\partial p_j}\right)_{\{p_z^1 - p_z^2, \forall z \neq k,j\}} - \left(\frac{\partial p_k^2}{\partial p_j}\right)_{\{p_z^1 - p_z^2, \forall z \neq k,j\}}}{\left(\frac{\partial p_k^1}{\partial p_i}\right)_{\{p_z^1 - p_z^2, \forall i \neq k,i\}} - \left(\frac{\partial p_k^2}{\partial p_i}\right)_{\{p_z^1 - p_z^2, \forall i \neq k,i\}}}. \tag{3.56}$$

obtained using Eq. 3.46 with $\pi_p = p_i$ and $\pi_g = p_j$. If the utility is a first order homogeneous function then Eq. 3.56 simplifies to:

$$\frac{\partial p_i}{\partial p_j}_{\{p_z^1 = p_z^2, \forall z \neq i,j\}} = -\frac{\frac{x_j^1}{x_z^1} - \frac{x_j^2}{x_z^2}}{\frac{x_i^1}{x_z^1} - \frac{x_i^2}{x_z^2}}. \tag{3.57}$$

In the consumer system, the phase transition occurs as the consumer exchanges goods with the market at constant prices. Thus, a phase transition in consumer theory, can be thought of as a transition between two separate points in the utility function, motivated by an increasing (or decreasing) endowment:

$$w \equiv w^1 + w^2 = \alpha w + (1-\alpha) w, \tag{3.58}$$

where α is the fraction of w spent in phase 1. The aggregate amounts of each product are given by the *Consumer Lever Rule*: $p_i x_i = p_i x_i^1 + p_i x_i^2 = \alpha w \mathcal{X}_i^1 + (1-\alpha) w \mathcal{X}_i^2$, where

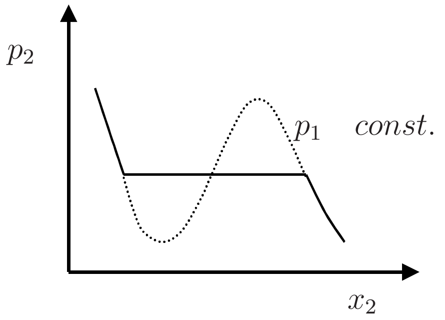

Figure 3.3: First Order Phase Transition in the Consumer.

$\mathcal{X}_i^1, \mathcal{X}_i^2$ are the equilibrium amounts of endowment spent on x_i^k per unit of endowment spent in phase k.

3.12 Conclusions

We have contributed to the unification of knowledge between Equilibrium Thermodynamics and Neoclassical Microeconomics by building a formalism common to both fields (Tab. 3.6 and 3.7). This general formalism includes (1) a derivation of a general relation between non-dimensional elasticities (Eq. 3.32 to Eq. 3.34) and (2) a derivation of the general formalism of first order phase transitions including a Generalized Clapeyron Equation (Eq. 3.46).

We obtained the following results in thermodynamics: (1) a relation between the non-dimensional thermodynamic coefficients and the change in Legendre transforms which highlights the importance of the non-dimensional coefficients in thermodynamics (Sec. 3.7), (2) the distinction between mathematical integrability and the optimization (Sec. 3.10) and (3) the generalization of the Clapeyron Equation (Eq. 3.53 and Eq. 3.54).

We obtained the following results in economics: (1) the definition of irreversibility in economic behavior (Sec. 3.4), (2) the clarification that the Engel curve and the offer curve are not descriptions of real processes dictated by the maximization of utility at constant endowment (Sec. 3.5), (3) a relation between elasticities (Eq. 3.39 to 3.41), (4) the proof that *Giffen Goods* do not exist in a stable equilibrium (Sec. 3.9), (5) the establishment that ‘economic integrability’ is equivalent to the Generalized Le Chatelier Principle (Sec. 3.10) and (6) the definition of a phase transition of first order characterized by an infinite own price elasticity of demand (Sec. 3.11). The importance of phenomena similar to phase transitions in economics has been recently highlighted for financial markets [21, 37] and

	General Formalism	**Thermodynamic Formalism**
Fundamental Function	$y(x_1, \ldots, x_n)$	$S(U^1, U^2, V^1, V^2, N_1^1, \ldots, N_r^2)$
Extensive Variables	x_i	U^j, V^j, N_i^j
Intensive Variables	π_i	$\frac{1}{T^j}, \frac{P^j}{T^j}, -\frac{\mu_i^j}{T^j}$
Duality Function	$x_1(y, x_2, \ldots, x_n)$	$U(S^1, S^2, V^1, V^2, N_1^1, \ldots, N_r^2)$
Irreversibility	Increase in y at constant g^z	Increase in S at constant U, V, N_i
Value Function	$y^*(k_1, \ldots, k_l)$	$S^*(U, V, N_1, \ldots, N_r)$
Legendre Transforms	$\varphi(x_1, \ldots, \pi_i, \ldots, x_n)$	$F = U - TS$ $H = U + PV$ $G = U - TS + PV$
Elasticities	$q_{\Pi,X}^{ij}$	$\alpha, c_v, c_P, \kappa_s, \kappa_T$
Maxwell Relations		$\frac{c_P}{c_v} = \frac{\kappa_T}{\kappa_s}$
Le Chatelier Principle	$0 > q_{\{x_i, \forall i \neq k\}}^{kk} > \ldots$ $> q_{x_j, \{\pi_i, \forall i \neq k, j\}}^{kk} > q_{\{\pi_i, \forall i \neq k\}}^{kk}$	$c_P > c_v > 0$ and $\kappa_T > \kappa_s > 0$
Equations of State	$\pi_i(x_1, \ldots, x_n)$	$T(S, V, N_1, \ldots, N_r)$ $P(S, V, N_1, \ldots, N_r)$ $\mu_i(S, V, N_1, \ldots, N_r)$
Integrability	Hessian matrix is: symmetric and negative semidefinite	Maxwell Relations Constraints on elasticities
Phase transition	$q_{\{\pi_i, \forall i \neq j\}}^{jj} = \infty$	$c_P = \infty, \alpha = \infty, \kappa_T = \infty$
Maxwell construction	π_k: $\int_{\pi_k^1}^{\pi_k^2} x_k d\pi_k = 0$	$\int_{P^1}^{P^2} V dP = 0$

Table 3.6: Table of Correspondences I.

for an Ising economy [3]. With the general formalism provided in this chapter for the first order phase transition, this concept can be applied more rigorously and extended to other fields of economics.

Differences between the formalism of thermodynamics and the microeconomic formalism are: (1) the fundamental equation in thermodynamics must be a homogeneous first order equation because entropy is additive over the subsystems while in microeconomics the utility is not [12], (2) the integrability problem is solved in microeconomics by imposing that the consumer is always rational (which is not always empirically true) while in thermodynamics it is solved by imposing the second law (which has always been em-

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[12] In the field of Nonextensive Thermodynamics entropy is no longer a homogeneous first order function.

	General Formalism	**Economic Formalism**
Fundamental Function	$y(x_1, \ldots, x_n)$	$U(x_1, \ldots, x_n)$
Extensive Variables	x_i	x_i
Intensive Variables	π_i	MU_i
Duality Function	$x_1(y, x_2, \ldots, x_n)$	$x_1(U, x_2, \ldots, x_n)$ $w(x_1, \ldots, x_n)$
Irreversibility	Increase in y at constant g^z	Increase in U at constant w
Value Function	$y^*(k_1, \ldots, k_l)$	$U^*(w, p_1, \ldots, p_n)$
Legendre Transforms	$\varphi(x_1, \ldots, \pi_i, \ldots, x_n)$	$\Psi = w - \sum\limits_{i=1,l} x_i p_i$
Elasticities	$q^{ij}_{\Pi,X}$	$\varepsilon_{\{p_k,\forall k\neq i\}}, \varepsilon_{\{x_k,\forall k\neq j\}}$ $e_{\{p_k,\forall k\neq i\}}, e_{\{x_k,\forall k\neq j\}}, \mathfrak{e}_{\{p_k,\forall k\neq i\}}$
Maxwell Relations	$\frac{\varepsilon_{p_1}}{\varepsilon_{p_2}} = \frac{\varepsilon_{x_1}}{\varepsilon_{x_2}}$	
Le Chatelier Principle	$0 > q^{kk}_{\{x_i,\forall i\neq k\}} > \ldots$	$0 > \varepsilon_{x_k} > \varepsilon_{p_k}$
Equations of State	$\pi_i(x_1, \ldots, x_n)$	$p_j(x_1, \ldots, x_n)$
Integrability	Hessian matrix is: symmetric and negative semidefinite	Antonelli's integrability conditions Constraints on elasticities or economic integrability
Phase transition	$q^{jj}_{\{\pi_i,\forall i\neq j\}} = \infty$	$\varepsilon_{\{p_k,\forall k\neq i\}} = \infty, e_{\{p_k,\forall k\neq i\}} = \infty$ $\mathfrak{e}_{\{p_k,\forall k\neq i\}} = \infty$
Maxwell construction	π_k: $\int\limits_{\pi_k^1}^{\pi_k^2} x_k d\pi_k = 0$	$\int\limits_{p_k^1}^{p_k^2} x_k dp = 0$

Table 3.7: Table of Correspondences II.

pirically true), (3) there is no equivalent to the Expenditure Duality in thermodynamics because thermodynamic intensive variables do not all have the same meaning and (4) the composite vs. simple systems issue only exists in thermodynamics because the entropy is only defined in equilibrium while utility is defined out of equilibrium. The measurement of the entropy in a thermodynamic system out of equilibrium implies that: (1) the system be divided into subsystems where the entropy is defined, i.e., subsystems in equilibrium and (2) the total entropy of the composite system be obtained by summing up the entropies of the subsystems. In contrast, the measurement of the utility out of equilibrium is straightforward because utility is defined for all consumption baskets.

Among the works cited in the introduction on the analogy between equilibrium thermodynamics and neoclassical microeconomics we would like to emphasize the contributions made by Rozonoer [23, 24, 25], Samuelson [27, 26] and Smith and Foley [30]. In this chapter we follow the same approach that is followed in these works considering that the entropy is formally analogous to the utility. Samuelson applies Le Chatelier Principle to economic systems. Rozonoer establishes an analogy between mechanisms of resource exchange and allocation in thermodynamics and economics. This author also obtains a version of the Le Chatelier Principle, although it is less general then the one obtained here. Smith and Foley depart from the three axioms for the mathematical representation of thermodynamic and economic systems (the three laws of thermodynamics). These authors obtain as the second law for the consumer theory a definition of irreversibility in economic behavior similar to the one proposed in this chapter, although our definition of irreversibility is valid only for a constant endowment (constant energy for a thermodynamic system). We believe that this constraint is necessary in the definition of irreversibility because if the consumer is forced to decrease his endowment, e.g., due to a new tax, then he might find optimal to reverse a trade that has increased his utility in the past.

Future work on the topic of equilibrium econophysics should encompass: (1) the derivation of first order phase transitions for the consumer theory with other constraints and between different utility functions, (2) the derivation of second-order phase transitions, (3) the establisment of a relation between consumer theory and social welfare analogous to the relation between statistical physics and macrothermodynamics and (4) the improvement of consumer theory to include thermodynamic irreversibility (building on the work of Sousa and Domingos [31]).

3.13 Appendices

3.13.1 Appendix I

The composite system can have an arbitrary number of subsystems; in this chapter, we consider only the simplified case of two subsystems. Each subsystem is a homogeneous system, i.e., it has a uniform temperature, pressure and chemical potentials for each chemical species. Each subsystem is a simple system.

According to Callen's postulate III [4], the entropy of a composite system is additive over the constituent subsystems, i.e., $S = \sum_{j=1}^{2} S^i$, where the entropy of each subsystem is a function of its extensive variables $S^j(U^j, V^j, N_1^j, \ldots, N_r^j)$. Thus, the entropy of the system is $S(U^1, U^2, V^1, V^2, N_1^1, N_1^2, \ldots, N_r^1, N_r^2)$. Applying the same reasoning to the internal energy, it can be concluded that $U(S^1, S^2, V^1, V^2, N_1^1, N_1^2, \ldots, N_r^1, N_r^2)$.

The enthalpy of subsystem j is $H^j = U^j + P^jV^j$ and the enthalpy of the composite system is $H = \sum_{j=1}^{2} H^j = \sum_{j=1}^{2} U^j + P^jV^j$. If the intensive variable is the same for both subsystems, i.e., $P^1 = P^2$ then $H = \sum_{j=1}^{2} U^j + PV^j = U + PV$. The same reasoning can be applied to the other Legendre transforms to obtain the expressions given in sec. 3.6.

Elasticities defined in sec. 3.7 can always be used to characterize simple systems. In the case of composite systems: (1) α, c_P and κ_T are adequate for composite systems with homogeneous temperature and pressure, (2) κ_s for composite systems with homogeneous pressure and (3) c_v for composite systems with homogeneous temperature.

Equations of state can describe: (1) composite systems in equilibrium or (2) each subsystem separately.

3.13.2 Appendix II

The Hessian of the Lagrangean function is given by:

$$\begin{bmatrix} \mathcal{L}_{11} & \cdots & \mathcal{L}_{1n} & g_1^1 & \cdots & g_1^m \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \mathcal{L}_{n1} & \cdots & \mathcal{L}_{nn} & g_n^1 & \cdots & g_n^m \\ g_1^1 & \cdots & g_1^m & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ g_n^1 & \cdots & g_n^m & 0 & \cdots & 0 \end{bmatrix},$$

where $\mathcal{L}_{ij} = \frac{\partial^2 \mathcal{L}}{\partial x_j \partial x_i}$ and $g_j^i = \frac{\partial g^i}{\partial x_j}$ [13].

3.13.3 Appendix III

A more detailed deduction of the relation between elasticities given by Eq. 3.32 is presented below. Relations given by Eq. 3.33 to Eq. 3.34 are obtained in a similar manner. Starting from

$$\left(\frac{\partial x_k}{\partial \pi_k}\right)_{\{\pi_i, \forall i \neq k\}} = \left(\frac{\partial x_k}{\partial \pi_k}\right)_{x_j, \{\pi_i, \forall i \neq k, j\}} + \left(\frac{\partial x_k}{\partial x_j}\right)_{\{\pi_i, \forall i \neq j\}} \left(\frac{\partial x_j}{\partial \pi_k}\right)_{\{\pi_i, \forall i \neq k\}} \tag{3.59}$$

and (1) multiplying by $\left(\frac{\partial x_j}{\partial \pi_j}\right)_{\{\pi_i,\forall i\neq j\}}$ and (2) using the Maxwell relation $\left(\frac{\partial x_k}{\partial \pi_j}\right)_{\{\pi_i,\forall i\neq j\}} = \left(\frac{\partial x_j}{\partial \pi_k}\right)_{\{\pi_i,\forall i\neq k\}}$ we obtain,

$$\begin{aligned}\left(\frac{\partial x_j}{\partial \pi_j}\right)_{\{\pi_i,\forall i\neq j\}}\left(\frac{\partial x_k}{\partial \pi_k}\right)_{\{\pi_i,\forall i\neq k\}} &= \\ = \left(\frac{\partial x_j}{\partial \pi_j}\right)_{\{\pi_i,\forall i\neq j\}}\left(\frac{\partial x_k}{\partial \pi_k}\right)_{x_j,\{\pi_i,\forall i\neq k,j\}} &+ \\ \left(\frac{\partial x_j}{\partial \pi_k}\right)_{\{\pi_i,\forall i\neq k\}}\left(\frac{\partial x_j}{\partial \pi_k}\right)_{\{\pi_i,\forall i\neq k\}} &. \end{aligned} \tag{3.60}$$

Eq. 3.32 is obtained by multiplying Eq. 3.60 by $\frac{\pi_k}{x_k}$ and rearranging.

The deduction of Eq. 3.35 is presented next. The differential of the extensive variable x_k can be written as:

$$dx_k = \frac{\partial x_k}{\partial \pi_1}d\pi_1 + \ldots + \frac{\partial x_k}{\partial \pi_n}d\pi_n. \tag{3.61}$$

Starting with Eq.3.61 the following steps are taken: (1) the Maxwell relation, $\left(\frac{\partial x_i}{\partial \pi_k}\right)_{\{\pi_j,\forall j\neq k\}} = \left(\frac{\partial x_k}{\partial \pi_i}\right)_{\{\pi_j,\forall j\neq i\}}$ (Tab 3.2) is used to replace the partial derivatives, (2) the expression is differentiated in relation to π_k with x_i constant and (3) the expression is multiplied by $\frac{\pi_k}{x_k}$ and the following equation is obtained:

$$\begin{aligned}\frac{\pi_k}{x_k}\left(\frac{\partial x_k}{\partial \pi_k}\right)_{\{x_i,\forall i\neq k\}} &= \\ \frac{\pi_k}{x_k}\left(\frac{\partial x_1}{\partial \pi_k}\right)_{\{\pi_i,\forall i\neq k\}}\left(\frac{\partial \pi_1}{\partial \pi_k}\right)_{\{x_i,\forall i\neq k\}} &+ \\ \ldots + \frac{\pi_k}{x_k}\left(\frac{\partial x_n}{\partial \pi_k}\right)_{\{\pi_i,\forall i\neq k\}}\left(\frac{\partial \pi_n}{\partial \pi_k}\right)_{\{x_i,\forall i\neq k\}} &. \end{aligned} \tag{3.62}$$

Using the elasticity given by Eq. 3.27, Eq. 3.62 can be written:

$$\begin{aligned} q^{kk}_{\{x_i,\forall i\neq k\}} = \frac{x_1}{x_k} q^{1k}_{\{\pi_i,\forall i\neq k\}}\left(\frac{\partial \pi_1}{\partial \pi_k}\right)_{\{x_i,\forall i\neq k\}} &+ \\ \ldots + \frac{x_n}{x_k} q^{nk}_{\{\pi_i,\forall i\neq k\}}\left(\frac{\partial \pi_n}{\partial \pi_k}\right)_{\{x_i,\forall i\neq k\}} &. \end{aligned} \tag{3.63}$$

With the partial derivatives replaced by

$$\left(\frac{\partial \pi_j}{\partial \pi_k}\right)_{x_i\neq k} = -\frac{\pi_j q^{jk}_{\pi_j,\{x_i,\forall i\neq k,j\}}}{\pi_k q^{jj}_{\pi_k,\{x_i,\forall i\neq k,j\}}}, \tag{3.64}$$

obtained using Eq. 3.27, Eq. 3.63 simplifies to Eq. 3.35.

3.13.4 Appendix IV

A simple and direct demonstration of the Euler Equation is presented by Callen [4, pp. 59], where Equation $y(\lambda x_1, \dots, \lambda x_n) = \lambda y(x_1, \dots, x_n)$ is differentiated with respect to λ and then λ is set to 1.

The Gibbs-Duhem Equation, $0 = x_1 d\pi_1 + \dots + x_n d\pi_n$, is obtained by combining the differential of the Euler Equation, $dy = \pi_1 dx_1 + \dots + \pi_n dx_n + x_1 d\pi_1 + \dots + x_n d\pi_n$, with the fundamental equation $dy = \pi_1 dx_1 + \dots + \pi_n dx_n$.

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Chapter 4

The thermodynamics of organisms in the context of DEB theory

Abstract

We carry out a thermodynamic analysis to an organism. It is applicable to any type of organism because 1) it is based on a thermodynamic formalism applicable to all open thermodynamic systems and 2) uses a general model to describe the internal structure of the organism - the Dynamic Energy Budget Model. Our results on the thermodynamics of DEB organisms are the following. (1) Thermodynamic constraints for the following types of organisms: (a) aerobic and exothermic, (b) anaerobic and exothermic and (c) anaerobic and endothermic; showing that anaerobic organisms have a higher thermodynamic flexibility. (2) A way to compute the changes in the enthalpy and in the entropy of living biomass that accompany changes in growth rate solving the problem of evaluating the thermodynamic properties of biomass as a function of the amount of reserves. (3) Two expressions for Thornton's coefficient that explain its experimental variability and theoretically underpin its use in metabolic studies. (4) A new mechanism that organisms in non steady-state use to rid themselves of internal entropy production: 'dilution of entropy production by growth'. To demonstrate the practical applicability of DEB theory to quantify thermodynamic changes in organisms we use published data on *Klebsiella aerogenes* growing aerobically in a continuous culture. We obtain different values for molar entropies of the reserve and the structure of *Klebsiella aerogenes* proving that the reserve density concept of DEB theory is essential in discussions concerning (a) the relationship between organization and entropy and (b) the mechanism of storing entropy in new biomass. Additionally, our results suggest that the entropy of dead biomass is significantly

different from the entropy of living biomass.

Keywords: Organism, Thermodynamics, Dynamic Energy Budget Theory, Entropy, Enthalpy, Thornton's coefficient.

4.1 Introduction

Many thermodynamic analyses of living organisms and cells have been made. Demirel et al.[10], for example, used thermodynamics to describe the coupled phenomena of transport and chemical reactions that take place inside living systems; Battley analyzed the entropy change accompanying the growth of *E. coli* [2] and the growth of *Saccharomyces cerevisiae* [5]; Stockar et al. [31, 32] analyzed the internal entropy production in some micro-organisms; Esener et al. [12] studied the energetics of *Klebsiella aerogenes*; Duboc et al. [11] evaluated the thermodynamic efficiency of *Saccharomyces cerevisae*; Qian and Beard [29] introduced a thermodynamic formalism to study metabolic biochemical reaction networks, etc.

The thermodynamic analyses mentioned use equations that describe chemical reactions that take place inside an organism as the model describing the organism's behavior; examples of these aggregated chemical reactions are given in Battley[5, Table 2] for some microorganisms. Because these models need a considerable amount of data they are not useful in thermodynamic analyses made of more complex organisms. Even for microorganisms these models present problems because they do not give a mechanistic explanation of many of the energetic aspects of an organism's growth process; this is patent in the ad-hoc explanations given for the empirical results.

The thermodynamic analyses that have been made would benefit from a general theory underlying the description of the energetic fluxes in order to build up solid knowledge about organism's metabolism. The Dynamics Energy Budget (DEB) theory is the most general non-species-specific theory of this kind [22, 23, 28]. It consists of a set of simple, mechanistically inspired rules that fully specify the uptake and use of mass and energy by an organism. The frequently applied classical models by Monod and Marr-Pirt on bacterial growth, and the well-known model by Droop for nutrient limited growth of unicellular algae are all special cases of DEB theory. DEB theory also considers phenomena of a complexity well beyond these simple models, including simultaneous nutrient limitation, adaptation, co-metabolism, flocculated growth, product formation, aging and syntrophy.

Here, we will carry out a thermodynamic analysis of an organism using 1) the most general framework of non-equilibrium thermodynamics applicable to all open thermodynamic systems (de Groot and Mazur [19], Bejan [7] and Moran et al. [26]) and 2) the knowledge of its internal dynamics given by DEB theory.

This chapter is organized as follows. In section 4.2 we begin by defining the DEB thermodynamic system, i.e., the mass and energy flows in the organism and the dynamics of its state variables. This is followed by a thermodynamic analysis of the organism in section 4.3. This analysis uses the mass, energy and entropy balances together with DEB to obtain the thermodynamic constraints imposed on different types of organisms and to discuss the use of Thornton's coefficient. In Section 4.4 a thermodynamic characterization of *Klebsiella aerogenes* is done using published data from chemostat experiments. Section 4.5 concludes.

4.2 Thermodynamic System

To simplify our analysis, we focus on a single-reserve, single-structure heterotrophic that lives on a single substrate. It is a V1 morph, i.e., an organism whose surface area is proportional to volume. Extensions to include more substrates, reserves and/or structures have been formulated in the DEB theory to include autotrophs and nutritional details [22]. However, such extensions do not pose new thermodynamic problems. Appendix 4.6.1 presents an explanation of the notation used throughout the chapter.

Fig. 5.1 presents a scheme, according to DEB theory, for an asexually propagating heterotrophic organism [1]. The simplest DEB model delineates one reserve, E, with M_E C-moles, and one structure, V, with M_V C-moles; the chemical composition of each is assumed to be constant (the strong homeostasis assumption). This simplifying assumption combines nicely with the idea that the enzymes that catalyse chemical transformations in the organism do so in a constant chemical environment, which is essential for full control. Reserve has the dual role of providing both energy and essential compounds for growth, maintenance, development and reproduction.

The incoming and outgoing fluxes through the outer surface of the system can be divided into organic (food, X and products, P), and mineral (CO_2, H_2O, O_2, and nitrogenous waste, N_{waste}) compounds. The energy flow of the food uptake per C-mol of structure $\dot{p}_X$, enters and is transformed into an assimilation energy flux per C-mol of structure, $\dot{p}_A$, that goes into the reserves and into products, P, that are excreted. The catabolic

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[1] The simplifications chosen are suitable for our empirical application.

energy flux, $\dot{p}_C$, i.e., the rate per C-mol of structure, at which the organism mobilizes its reserve for metabolic purposes [2], is partitioned between growth, $\dot{p}_G$, and maintenance, $\dot{p}_M$, i.e.,

$$\dot{p}_C = \dot{p}_M + \dot{p}_G. \tag{4.1}$$

Maintenance includes a variety of requirements, such as the turnover of chemical compounds of structure (e.g. proteins), the maintenance of concentration gradients across membranes, the maintenance of defense systems (e.g. the immune system), activity (including behavior), the heating of the body to a near constant temperature (endotherms only) and osmotic work (especially freshwater organisms) [22]. Growth is defined as the increase of structure; body weight has contributions from both reserve and structure.

Ellipses in Fig. 5.1 are idealized reactors where anabolic and catabolic processes take place. These transformations occur all over the organism, rather than at specific sites. Consequently, the idealized reactors are the transformations themselves. These processes are characterized by constant conversion efficiencies between mass flows, y_{*1*2}, i.e., the number of moles of $*1$ needed to produce one mol of $*2$. In the assimilation reactor food is converted into reserve, y_{XE}, and in the growth reactor reserve is converted into structure, y_{EV}.

The ratio $m_E \equiv M_E/M_V$ is the reserve density. For any constant food level, $X = X^* > 0$, there is a reserve density, m_E^*, that remains constant along the growth process. Furthermore $\lim_{X^* \to \infty} m_E^* \equiv m_{Em}$ where m_{Em} is the maximum reserve density (the weak homeostasis assumption).

We now quantify the dynamics of the state variables structure and reserve. The amount of structure and reserve and the flows in the organism are measured in mass and Gibbs energy and the conversion between them is done using chemical potentials: the chemical potential of food, μ_X, converts the flow of food per C-mol of structure, j_X, to $\dot{p}_X$; the chemical potential of reserve, μ_E, converts the flow of reserve that exits the assimilation reactor to $\dot{p}_A$ and the flow of reserve that exits the reserve compartment to $\dot{p}_C = \dot{p}_M + \dot{p}_G$.

The change in C-moles of reserve per C-mol of structure is:

$$j_E \equiv \frac{1}{M_V}\frac{dM_E}{dt} = \frac{\dot{p}_A - \dot{p}_C}{\mu_E}, \tag{4.2}$$

because the reserve is continuously used (catabolic power) and replenished (assimilation power). With Eq. 4.2, the reserve density dynamics is

$$\frac{dm_E}{dt} \equiv \frac{d(M_E/M_V)}{dt} = \frac{\dot{p}_A - \dot{p}_C}{\mu_E} - m_E\frac{1}{M_V}\frac{dM_V}{dt}, \tag{4.3}$$

---

[2] Catabolism has a somewhat different meaning in the biochemistry literature.

where the last term on the right hand side is the dilution by growth.

To further evaluate the reserve dynamics we need to quantify feeding and assimilation. The food uptake per C-mol of structure is given by $j_X = f j_{Xm}$ where f is the scaled functional response and j_{Xm} is the maximum food uptake per C-mol of structure, i.e., the food uptake that would occur at abundant food availability. The assimilation energy flow per C-mol of structure is

$$\dot{p}_A = \frac{j_X}{y_{XE}} \mu_E, \tag{4.4}$$

where $\frac{j_X}{y_{XE}}$ is the reserve flow that exits the assimilation reactor per C-mol of structure.

The reserve dynamics can be further deduced considering 1) that the catabolic power is independent of the food availability, 2) that the mobilization of reserves does not depend on how they are partitioned among aggregates with different chemical compositions and 3) the weak homeostasis assumption (for details on the derivation see Appendix 4.6.2). The reserve dynamics is then

$$\frac{dm_E}{dt} = \dot{k}_E \left(f m_{Em} - m_E \right), \tag{4.5}$$

where $\dot{k}_E$ is the maximum reserve turnover rate:

$$\dot{k}_E = \frac{j_{Xm}/y_{XE}}{m_{Em}}. \tag{4.6}$$

The parameter $\dot{k}_E$ is a turnover rate because it is the ratio between the maximum flow of C-moles of reserve into the 'reserve compartment', $j_{Xm}/y_{XE} M_V$, and the maximum amount of C-moles of reserve kept in the 'reserve compartment', $m_{Em} M_V$.

By combining Eq. 4.3 with Eq. 4.5 the catabolic power simplifies to:

$$\dot{p}_C = \mu_E m_E \left(\dot{k}_E - \frac{1}{M_V} \frac{dM_V}{dt} \right). \tag{4.7}$$

To evaluate the dynamics of the structure we need to quantify maintenance and growth. The maintenance energy flow per C-mol of structure is

$$\dot{p}_M = \dot{k}_M y_{EV} \mu_E, \tag{4.8}$$

where $\dot{k}_M y_{EV}$ is the reserve flow that exits the reserve for maintenance purposes per C-mol of structure and $\dot{k}_M$ is the maintenance rate coefficient. The growth energy flow per C-mol of structure is

$$\dot{p}_G = j_V y_{EV} \mu_E, \tag{4.9}$$

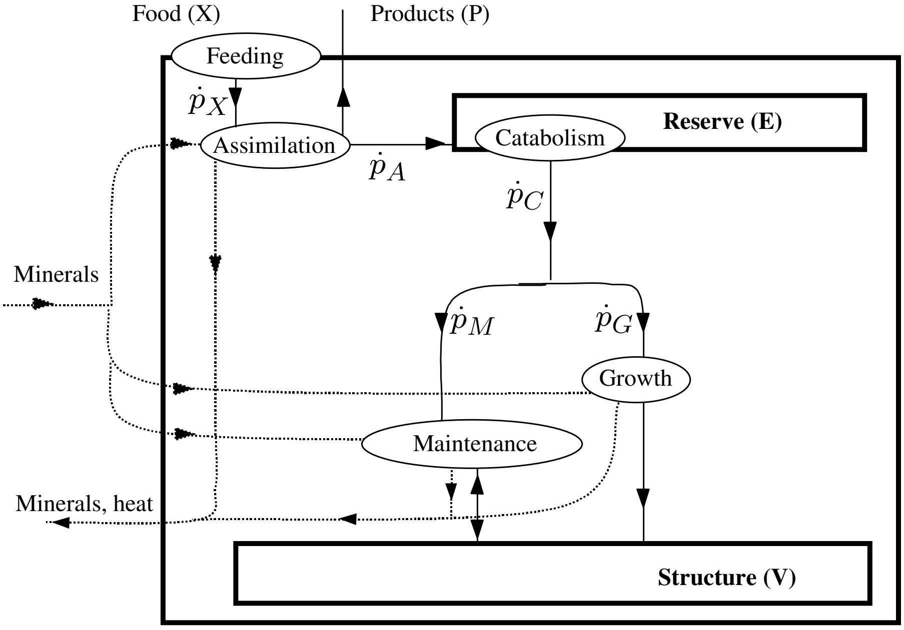

Figure 4.1: Schematization of an asexually propagating heterotrophic organism following DEB theory. Boxes represent boundaries. Ovals represent chemical reactors. Lines represent mass and energy flows: $\dot{p}_X$ has the chemical composition of food; $\dot{p}_A$, $\dot{p}_C$, $\dot{p}_G$ and $\dot{p}_M$ have the chemical composition of reserve and the flow that goes from the growth reactor to the structure compartment has the chemical composition of structure.

	Compound
X	Food
P	Products
E	Reserve
V	Structure
W	Biomass
$\mathcal{O}$	class of organic compounds (X, P, E, V)
$\mathcal{M}$	class of mineral compounds (CO_2, H_2O, O_2, N_{waste})

Table 4.1: List of compounds.

where $j_V y_{EV}$ is the flow that exits the reserve for growth purposes per C-mol of structure and j_V is the molar flow of structure.

The dynamics of structure

$$j_V \equiv \frac{1}{M_V}\frac{dM_V}{dt} = \frac{\dot{p}_G}{y_{EV}\mu_E} = \frac{(\dot{k}_E\frac{m_E}{m_{Em}} - \dot{k}_M g)}{(\frac{m_E}{m_{Em}} + g)}, \tag{4.10}$$

is obtained by combining Eq. 4.1, Eq. 4.8, Eq. 4.9, and Eq. 4.7, where the investment ratio, g, is a dimensionless quantity given by

$$g \equiv y_{EV}/m_{Em}, \tag{4.11}$$

that stands for the ratio between the number of moles of reserve allocated to growth per mole of structure and the maximum number of moles of reserve allocated to maintenance plus growth per mole of structure. At constant food the dynamics of structure simplifies to:

$$j_V = (\dot{k}_E f - \dot{k}_M g)/(f + g), \tag{4.12}$$

because the weak homeostasis assumption implies that $\frac{dm_E}{dt} = 0$.

4.3 Thermodynamic Analysis

We now formalise the thermodynamic analysis. See Table 4.1 for a list of compounds.

If the mole numbers of each compound, the total energy and the total entropy of the organism are constant, the organism is in steady state. In this state there is still a continuous flow of matter, energy and entropy through the system from and to external reservoirs. This is implied by maintenance requirements. Here, we will consider that the organism is not in steady state because our life cycle perspective of an individual comes with the necessity to consider changes in amounts of reserve and structure, both in mass and energy aspects.

The strong homeostasis assumption justifies one of the main simplifications used in the thermodynamic analysis: the molar chemical compositions, internal energies, enthalpies and entropies of reserve and structure are taken to be constant, independent of the reserve density. In general, we consider that the chemical composition of biomass (structure plus reserve) can change; this implies that the molar thermodynamic properties of biomass can also change. Whenever the reserve density is constant, the chemical composition of biomass and its molar thermodynamic properties are also constant.

4.3.1 Mass Balance Equation

Most of the dry mass of biological systems consists of proteins, lipids, carbohydrates and nucleic acids. The major chemical elements in the covalently bounded compounds are carbon, C, hydrogen, H, oxygen, O, nitrogen, N, phosphorus and sulphur. The first four elements stand for more than 96 % of the total dry mass [27], so we focus on these elements only. A 'molecule' of structure is denoted by $\mathrm{CH}_{n_{HV}}\mathrm{O}_{n_{OV}}\mathrm{N}_{n_{NV}}$, a 'molecule' of reserve by $\mathrm{CH}_{n_{HE}}\mathrm{O}_{n_{OE}}\mathrm{N}_{n_{NE}}$, where the chemical index n_{ij} is the number of atoms of element i per atom of carbon in compound j. The mass balance equation for the organism is written on a molar basis for each element because there is no conservation of compounds due to the chemical transformations inside the organism. The mass balance equation is:

$$0 = \boldsymbol{n}_{\mathcal{M}}\dot{\boldsymbol{J}}_{\mathcal{M}} + \boldsymbol{n}_{\mathcal{O}}\dot{\boldsymbol{J}}_{\mathcal{O}} \tag{4.13}$$

where $\dot{\boldsymbol{J}}_{\mathcal{M}}$ is the vector with the molar fluxes of the minerals ($\dot{J}_{CO_2}$, $\dot{J}_{H_2O}$, $\dot{J}_{O_2}$, $\dot{J}_{N_{waste}}$), $\dot{\boldsymbol{J}}_{\mathcal{O}}$ is the vector with the molar fluxes of the organics ($\dot{J}_X$, $\dot{J}_P$, $-\dot{J}_V$, $-\dot{J}_E$), $\boldsymbol{n}_{\mathcal{M}}$ is the matrix with the chemical composition of minerals and $\boldsymbol{n}_{\mathcal{O}}$ is the matrix with the chemical composition of organic compounds. Each entry in these matrices, n_{*1*2}, is the number of atoms of element $*1$ in compound $*2$.

The fluxes $\dot{J}_V \equiv \frac{d}{dt}M_V$ and $\dot{J}_E \equiv \frac{d}{dt}M_E$ are the change in C-mols of structure and reserve per unit time in the organism. The other fluxes, $\dot{J}_j$, mole numbers per unit time, are positive if they represent a net input into the thermodynamically defined organism and negative otherwise. In a heterotrophic organism CO_2 is usually but not always an output, O_2 is an input, H_2O is an output formed metabolically from other compounds, nitrogenous waste is an output, food is an input and products are an output. Eq. (4.13) states that, for each element, the rate of mole numbers accumulation inside the organism (structure and reserve), equals the inputs minus the outputs (other organic and mineral flows).

4.3.2 Energy Balance Equation

The energy balance equation quantifies the organism's accumulation of energy as the result of inputs minus outputs of energy fluxes. The energy fluxes (Joule/s) are the net heat flux, the net work flux and energy fluxes associated with input and output molar fluxes.

In this analysis mechanical work will be considered negligible. This is supported by Garby et al. [17], who state that 'the energy transfer as heat (in animals) is relatively large and directed outwards, while the energy transfer as work is small'.

The temperature of structure, reserve and outgoing products, T, is assumed constant and equal to the temperature of the body. We think this is a reasonable first approximation because chemical reactions inside the organism occur for a limited temperature range mainly due to enzymatic action [22]. Anyway this will probably be a better approximation for endotherms or for ectotherms in an environment where they are able to keep their temperature constant by moving.

This set of assumptions, i.e., a constant temperature of the organism, negligible mechanical work and incoming fluxes with a temperature similar to the organism's imply that the net heat released by the organism equals the net heat produced in all chemical reactions inside the organism. Chemical reactions taking place are the degradation of food and reserve material in order to obtain energy (synthesize ATP from ADP) and release nutrients, and the building up of reserve and new structural material with the nutrients and energy obtained.

Here, we apply the energy balance equation to aerobic and to anaerobic organisms. The distinction between these types of organisms is useful because there are simplifications applicable only to aerobic organisms (sections 4.3.2 and 4.3.3).

Energy Balance Equation: General Organism

With the simplifications that were mentioned in section 4.3.2, the energy balance of the entire thermodynamic system is

$$0 = \overline{\boldsymbol{h}}_{\mathcal{M}}^T \dot{\boldsymbol{J}}_{\mathcal{M}} + \overline{\boldsymbol{h}}_{\mathcal{O}}^T \dot{\boldsymbol{J}}_{\mathcal{O}} + \dot{P}_{T+} \tag{4.14}$$

where $\dot{P}_{T+}$ is the total released heat [3], $\overline{\boldsymbol{h}}_{\mathcal{M}}^T = \begin{pmatrix} \overline{h}_{CO_2} & \overline{h}_{H_2O} & \overline{h}_{O_2} & \overline{h}_{N_{waste}} \end{pmatrix}^T$ and $\overline{\boldsymbol{h}}_{\mathcal{O}}^T = \begin{pmatrix} \overline{h}_X & \overline{h}_P & \overline{h}_V & \overline{h}_E \end{pmatrix}^T$ and $\overline{h}_i$ is the molar enthalpy of compound i. The internal energy and the flow work linked to the input and output molar fluxes are lumped in the enthalpy.

Eq. 4.14 is the energy balance for a non-steady state organism defined according to DEB theory. This supports the use of direct calorimetry (the direct measurement of released heat) to assess enthalpy changes in organisms as referred by [31]: if the organism was completely burned then the net heat release plus the enthalpy of the combustion products would be equal to the organism's total enthalpy.

The enthalpy can be substituted by $\overline{h} = \overline{u} + P\overline{v} = \overline{g} + T\overline{s} = \mu + T\overline{s}$, which is obtained using the definition of Gibbs energy $\overline{g} = \overline{u} - T\overline{s} + P\overline{v}$ and the equality between Gibbs energy and chemical potential $g = \mu$ for a single component:

$$0 = (\boldsymbol{\mu}_{\mathcal{M}} + T\overline{\boldsymbol{s}}_{\mathcal{M}})^T \dot{\boldsymbol{J}}_{\mathcal{M}} + (\boldsymbol{\mu}_{\mathcal{O}} + T\overline{\boldsymbol{s}}_{\mathcal{O}})^T \dot{\boldsymbol{J}}_{\mathcal{O}} + \dot{P}_{T+} \tag{4.15}$$

where $\overline{s}_E$ is the molar entropy of the reserve, $\overline{s}_V$ is the molar entropy of the structure, $\overline{\boldsymbol{\mu}}_{\mathcal{M}}$ and $\overline{\boldsymbol{s}}_{\mathcal{M}}$ collect the values for the four minerals; $\overline{\boldsymbol{\mu}}_{\mathcal{O}}$ and $\overline{\boldsymbol{s}}_{\mathcal{O}}$ do that for the organic compounds, as before.

Energy Balance Equation: Aerobic Organism

We assume that reactors have negligible mass and are at pseudo steady state. An additional assumption that can also be made is based on Garby and Larsen [17] who consider, based on empirical knowledge, that for most important reactions in biological systems $T\Delta s$ is very small compared to Δh and therefore the enthalpy of the reaction $\Delta h_{reaction}$ is approximated using its Gibbs energy $\Delta g_{reaction}$, since at constant temperature $\Delta g = \Delta h - T\Delta s \simeq \Delta h$. This assumption is valid only for aerobic reactions but it is less stringent than that of Kooijman [22], where entropy is set to zero.

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[3] The heat follows the same sign convention as the mass flows: it is negative if the net input is negative, i.e., the heat released is negative

We apply the simplification that $T\Delta s$ is very small to the set of all reactors to obtain:

$$0 = \overline{\boldsymbol{s}}_{\mathcal{M}}^{T}\dot{\boldsymbol{J}}_{\mathcal{M}} + \overline{\boldsymbol{s}}_{\mathcal{O}}^{T}\dot{\boldsymbol{J}}_{\mathcal{O}}. \tag{4.16}$$

This equation can be disaggregated to

$$\overline{s}_V\dot{J}_V + \overline{s}_E\dot{J}_E = \overline{\boldsymbol{s}}_{\mathcal{M}}^{T}\dot{\boldsymbol{J}}_{\mathcal{M}} + \overline{s}_X\dot{J}_X + \overline{s}_P\dot{J}_P, \tag{4.17}$$

to emphasize that the entropy variation of an aerobic organism (left hand side), equals the net import of chemical entropy given by the right hand side of Eq. 4.17 [4]. With Eq. (4.17) we conclude that, for an aerobic organism, if weak homeostasis applies, i.e., reserve and structure are in constant proportions, then there is a positive net import of chemical entropy during an increase in biomass, a negative net import of chemical entropy during a decrease in biomass and a null net import at constant biomass (see the entries (1,1), (3,1) and (5,1) [5] in Table 4.2). If weak homeostasis does not apply and the structure and reserve molar entropies are different then an organism that is increasing its biomass could either have a positive or negative net import of chemical entropy. This is in accordance with Stockar and Liu [31] who concluded that microbial growth might result either from a positive or negative net import of chemical entropy.

The total entropy of an organism is easily computed if the molar entropy values and the chemical composition of biomass are known. Otherwise, Eq. 4.16 has to be integrated to obtain the total entropy of an organism as a function of total inputs and outputs from birth t_b until time t.

We apply the energy balance equation to the set of all reactors assuming that the reactors are in steady-state but that the organism as a whole is not. We obtain [6],

$$0 = \dot{Q}_{reactions} + \overline{\boldsymbol{\mu}}_{\mathcal{O}}^{T}\dot{\boldsymbol{J}}_{\mathcal{O}} + \overline{\boldsymbol{\mu}}_{\mathcal{M}}^{T}\dot{\boldsymbol{J}}_{\mathcal{M}} \tag{4.18}$$

where $\dot{Q}_{reactions}$ is the rate of the total heat release by all chemical reactions, since the work is null and the accumulation of energy is also null. Eq. 4.18 is equivalent to the energy balance equation presented in [22, p153] but it is applicable only to an aerobic organism. It would only be applicable to other organisms if entropies were set equal to zero in Eq. 4.15. This is not a reasonable assumption because it is equivalent to assuming

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[4] Chemical entropy is the entropy associated with mass.

[5] Entry is written as (line,column).

[6] We obtain this equation by summing the equations that describe the aggregate chemical reactions occurring in each reactor.

that the heat capacities of the various compounds including the minerals are null in the interval between the absolute temperatures 0 K and T. Eq. 4.18 can be disaggregrated to

$$\overline{\mu}_V \dot{J}_V + \overline{\mu}_E \dot{J}_E = \dot{Q}_{reactions} + \overline{\mu}_X \dot{J}_X + \overline{\mu}_P \dot{J}_P + \overline{\boldsymbol{\mu}}_{\mathcal{M}}^T \dot{\boldsymbol{J}}_{\mathcal{M}}. \tag{4.19}$$

4.3.3 Entropy Balance Equation

The entropy balance equation states that the change in entropy is equal to the entropy production inside the organism due to irreversible processes plus the net entropy flux associated with heat and mass fluxes. The entropy balance equation is different from the other balance equations because the accumulation of entropy inside the organism depends on the internal processes, which control the value of the entropy production.

Entropy Balance Equation: General Organism

The entropy balance for the organism is

$$0 = \dot{\sigma} + \frac{\dot{P}_{T+}}{T} + \overline{\boldsymbol{s}}_{\mathcal{M}}^T \dot{\boldsymbol{J}}_{\mathcal{M}} + \overline{\boldsymbol{s}}_{\mathcal{O}}^T \dot{\boldsymbol{J}}_{\mathcal{O}}, \tag{4.20}$$

which can be written as

$$\overline{s}_V \dot{J}_V + \overline{s}_E \dot{J}_E = \dot{\sigma} + \frac{\dot{P}_{T+}}{T} + \overline{\boldsymbol{s}}_{\mathcal{M}}^T \dot{\boldsymbol{J}}_{\mathcal{M}} + \overline{s}_X \dot{J}_X + \overline{s}_P \dot{J}_P, \tag{4.21}$$

where $\dot{P}_{T+}/T$ is the entropy exchange coupled with heat fluxes.

With Eq. 4.21 we conclude that for an anaerobic and exothermic organism [7] at constant biomass, if weak homeostasis applies then the organism can have a 1) positive or 2) negative net import of chemical entropy (see the entries (1,2) and (1,3) in Table 4.2). In case 1 (resp. case 2) $T\dot{\sigma} + \dot{P}_{T+} < 0$ (resp. $T\dot{\sigma} + \dot{P}_{T+} > 0$). In case 1 (resp. case 2), the organism will have a positive (resp. positive or negative) net import of chemical entropy when its biomass is increasing and a positive or negative (resp. negative) net import of chemical entropy when its biomass is decreasing (see the entries (3,2), (3,3) and (5,2), (5,3) in Table 4.2). For an aerobic and endothermic organism the net import of chemical entropy follows the same behaviour as in case 2 because $T\dot{\sigma} + \dot{P}_{T+} > 0$ (see the entries (1,4), (3,4) and (5,4) in Table 4.2).

Multiplying Eq. 4.20 by *T* and subtracting Eq. 4.15 we obtain

$$0 = \overline{\boldsymbol{g}}_{\mathcal{M}}^T \dot{\boldsymbol{J}}_{\mathcal{M}} + \overline{\boldsymbol{g}}_{\mathcal{O}}^T \dot{\boldsymbol{J}}_{\mathcal{O}} - \dot{\sigma} T, \tag{4.22}$$

---

[7] Exothermic (endothermic) organisms are organisms whose overall metabolism results in a negative (positive) net import of heat from the exterior.

where $\overline{g}_i$ is the molar Gibbs energy per mole of compound i. This equation can be disaggregated to

$$\overline{g}_V \dot{J}_V + \overline{g}_E \dot{J}_E + \dot{\sigma} T = \overline{\boldsymbol{g}}_{\mathcal{M}}^T \dot{\boldsymbol{J}}_{\mathcal{M}} + \overline{g}_X \dot{J}_X + \overline{g}_P \dot{J}_P. \tag{4.23}$$

to emphasize that the net import of Gibbs energy equals the rate of Gibbs energy change inside the organism plus an irreversibility production measure.

The net import of Gibbs energy by an anaerobic organism follows the same behaviour for exothermic and endothermic organisms (see Eq. 4.23). When the organism is either increasing its biomass or at constant biomass the net input of Gibbs energy is positive (see the entries (2,2), (2,3), (2,4), (4,2), (4,3) and (4,4)). When the organism is decreasing its biomass the net input of Gibbs energy is negative or positive (see the entries (6,2), (6,3) and (6,4)).

Entropy Balance Equation: Aerobic Organism

The results of the previous section can be further narrowed for aerobic organisms. Subtracting Eq. 4.16 from Eq. 4.20, we obtain

$$\dot{\sigma} = -\frac{\dot{P}_{T+}}{T}, \tag{4.24}$$

i.e., the rate of heat released by the aerobic organism equals minus an irreversibility production measure.

Therefore, since the second law tells us that entropy production is always positive, the total heat obtained from the organism is negative (released), which means that the sum of the processes of assimilation, dissipation and growth must be exothermic for aerobic life. The result of Kooijman in [22], i.e., 'the second law of thermodynamics implies that [each of] the processes of assimilation, dissipation and growth is exothermic', is obtained only by considering that entropies are null.

The second law only forbids that processes as a whole are endothermic when the organism is aerobic and the heat released by the organism is equal to the heat released in all chemical reactions. For example, using direct calorimetry, Stockar et al. [32, 25] showed the existence of a chemotroph whose overall metabolic process (assimilation plus dissipation plus growth) is endothermic. This rare type of overall metabolic process is called 'enthalpy retarded growth'.

With Eq. 4.19 and Eq. 4.24 we conclude that for an aerobic organism, if weak homeostasis applies then there is a positive net import of Gibbs energy at constant and at increasing biomass (see the entries (2,1) and (4,1) in Table 4.2). When the organism's

		Aerobic and exothermic	Anaerobic and exothermic		Anaerobic and endothermic
Constant Biomass	Chemical Entropy	0	+	-	-
	Gibbs energy	+	+	+	+
Increasing biomass	Chemical Entropy	+	+	+/-	+/-
	Gibbs energy	+	+	+	+
Decreasing biomass	Chemical Entropy	-	+/-	-	-
	Gibbs energy	+/-	+/-	+/-	+/-

Table 4.2: Net import of chemical entropy and Gibbs free energy in the overall metabolism for 1) exothermic aerobic organisms, 2) exothermic anaerobic organisms, and 3) endothermic anaerobic organisms. All organisms are at constant chemical composition (weak homeostasis). Organisms are either at constant, increasing or decreasing biomass. There are two columns for the anaerobic and exothermic organisms because 1) they can either have a positive or negative net import of chemical entropy at constant biomass (1^{st} line) and 2) this is related to their behavior when they are increasing or decreasing their biomass (3^{rd} and 5^{th} lines).

biomass is decreasing the net import of Gibbs energy is positive or negative (see the entry (6,1) in Table 4.2).

4.3.4 Constraints imposed by the second law and DEB Theory

In the previous sections we made predictions on the sign of the net input into the organism of Gibbs free energy and chemical entropy. These results are synthesized in Table 4.2. These predictions are made for aerobic exothermic organisms, anaerobic exothermic organisms and anaerobic endothermic organisms in a constant environment, for three situations: (1) steady-state (constant biomass), (2) non steady state with increasing biomass and (3) non steady state with decreasing biomass. The imposition of a constant environment is a sufficient condition for weak homeostasis, i.e., constant biomass molar entropy. Table 4.2 highlights the differences between aerobic and anaerobic organisms in a constant environment: (1) only anaerobic organisms can be endothermic, (2) only anaerobic organisms can have a net negative import of chemical entropy while increasing their biomass and (3) only anaerobic organisms can have a net positive import of chemical entropy while decreasing their biomass. Apparently, anaerobic organisms have a higher thermodynamic flexibility.

For steady state, the internal entropy production ($\dot{\sigma} > 0$) implies a relation between the heat and the chemical entropy exchange with the environment (see Eq. 4.21). Based on this, Stockar and Liu [31] distinguish different overall metabolisms: 'entropy neutral growth' (1^{st} column in Table 4.2), 'entropy driven growth' (3^{rd} and 4^{th} columns in Table 4.2) and 'entropy retarded growth' (2^{nd} column in Table 4.2) respectively for a null, negative or positive net import of chemical entropy.

However, the classification of Stockar and Liu [31] developed for the steady-state should not be used for the non steady state because it is misleading. An example is provided by aerobic organisms increasing their biomass. In this case they would be classified as 'entropy retarded' when the mechanism used to get rid of entropy production is heat dissipation only (see Eq. 4.24).

In non steady-states, organisms can get rid of internal entropy production by using an additional mechanism: accumulation of chemical entropy in new biomass. This mechanism can be called 'dilution of entropy production by growth'. The importance of the mechanism of accumulation of chemical entropy in biomass is fully dependent on the distinction introduced by DEB theory between reserve and structure. For an organism that is not in steady state but has a constant chemical composition (weak homeostasis) the capacity of this mechanism remains constant per C-mol of biomass increase (decrease) because the additional C-mol has the same entropy. In constrast, when the reserve density changes, the chemical composition of biomass and its entropy also change. Thus, the additional C-mol of biomass increase (decrease) has a different capacity to accumulate chemical entropy.

4.3.5 Calorimetry

Indirect Calorimetry

Indirect calorimetry is an empirical method of estimating heat production based on the measurements of gaseous exchanges and the nitrogenous waste flux [8] using multiple linear regression; see [3] or [24] for a good overview.

A theoretical underpinning for indirect calorimetry was provided by Kooijman [22]. Here, we obtained the linearity between the dissipated heat flux and the fluxes in a simpler and more direct way by using only a subset of DEB theory: the existence of strongly homeostatic reserve and structure.

We obtain the linear dependence between the mineral fluxes and the dissipated heat by combining Eq. 4.13 with Eq. 4.14,

$$\dot{P}_{T+} = (\overline{\boldsymbol{h}}_{\mathcal{O}}^{T}\boldsymbol{n}_{\mathcal{O}}^{-1}\boldsymbol{n}_{\mathcal{M}} - \overline{\boldsymbol{h}}_{\mathcal{M}}^{T})\dot{\boldsymbol{J}}_{\mathcal{M}}. \tag{4.25}$$

The coefficients that are obtained by linear regression are given by the expression in parentheses and can be computed without knowing any biochemical details. Only the chemical composition and the enthalpies of the reserve, the structure and the input and output products are needed. This result is a theoretical basis for the linear dependence between the mineral fluxes and the dissipated heat because it equates the total dissipating heat to a weighted sum of consumed dioxygen, produced carbon dioxide, nitrogen waste and water.

Thornton's rule

In the literature, Thornton's rule [33] is used to estimate heat production in aerobic organisms. This rule establishes a constant proportionality between the heat released in the combustion of organic compounds and the consumed oxygen: 444 kJ per mol of O_2 consumed. Recently the usefulness of this rule has been questioned by an experimental study made by Walsberg and Hoffman [34] because significant variations were obtained experimentally in the amount of heat released per mol of O_2 in a Kangoroo rat and a dove.

We now use DEB theory to obtain the conditions that keep constant the proportionality coefficient, h_{OT}, in the amount of heat released,

$$\dot{P}_{T+} = h_{OT}\dot{J}_{O_2}. \tag{4.26}$$

If the heat and the oxygen flows in Eq. 4.26 are written as functions of the organic fluxes using Eq. 4.13 and Eq. 4.25, then the proportionality coefficient is given by:

$$\begin{aligned} h_{OT} &= \frac{(\overline{\boldsymbol{h}}_{\mathcal{O}}^{T} - \overline{\boldsymbol{h}}_{\mathcal{M}}^{T}\boldsymbol{n}_{\mathcal{M}}^{-1}\boldsymbol{n}_{\mathcal{O}})\dot{\boldsymbol{J}}_{\mathcal{O}}}{\boldsymbol{n}_{\mathcal{M}}^{-1}(3,:)\boldsymbol{n}_{\mathcal{O}}\dot{\boldsymbol{J}}_{\mathcal{O}}} \\ &= \frac{\sum_{i=1}^{i=3}(\boldsymbol{h}_{\mathcal{O}}(i) - \overline{\boldsymbol{h}}_{\mathcal{M}}^{T}\boldsymbol{n}_{\mathcal{M}}^{-1}\boldsymbol{n}_{\mathcal{O}}(:,i))\dot{\boldsymbol{J}}_{\mathcal{O}}(i)}{\sum_{i=1}^{i=3}\boldsymbol{n}_{\mathcal{M}}^{-1}(3,:)\boldsymbol{n}_{\mathcal{O}}(:,i)\dot{\boldsymbol{J}}_{\mathcal{O}}(i)} \end{aligned} \tag{4.27}$$

where $i = 1$ is food, X, $i = 2$ is reserve, E, $i = 3$ is structure, V, $\boldsymbol{n}_{\mathcal{O}}(:,i)$ is column i of matrix $\boldsymbol{n}_{\mathcal{O}}$ and $\boldsymbol{n}_{\mathcal{M}}^{-1}(3,:)$ is the 3^{rd} line of matrix $\boldsymbol{n}_{\mathcal{M}}^{-1}$; it is the 3^{rd} line that appears because the 3^{rd} column of matrix $\boldsymbol{n}_{\mathcal{M}}$ has the chemical composition of O_2. Eq. 4.27 can be written as:

$$h_{OT} = \frac{\sum_{i=1}^{i=3}\dot{P}_{Ti+}\dot{\boldsymbol{J}}_{\mathcal{O}}(i)}{\sum_{i=1}^{i=3}\dot{J}_{O_2}(i)\dot{\boldsymbol{J}}_{\mathcal{O}}(i)} = \frac{\sum_{i=1}^{i=3}h_{OT_i}\dot{J}_{O_2}(i)\dot{\boldsymbol{J}}_{\mathcal{O}}(i)}{\sum_{i=1}^{i=3}\dot{J}_{O_2}(i)\dot{\boldsymbol{J}}_{\mathcal{O}}(i)}, \tag{4.28}$$

where $\dot{P}_{Ti+}$ is the heat released in the complete combustion of one C-mol of the organic compound i and $\boldsymbol{n}_{\mathcal{M}}^{-1}(3,:)\boldsymbol{n}_{\mathcal{O}}(:,i)$ is the number of O_2 moles consumed, $\dot{J}_{O_2}(i)$, in the complete combustion of a C-mol of the organic compound i. Because the heat released in the complete combustion of an organic compound is constant it can be written as the product of a constant h_{OT_i} and $\dot{J}_{O_2}(i)$.

With Eq. 4.28 the coefficient h_{OT} can be interpreted as a mean of the heats released per each mol of O_2 that would be spent in the complete combustion of each organic compound weighted by its net flow. For h_{OT} to be constant it has to be independent of the values of the organic flows $\boldsymbol{J}_{\mathcal{O}}(i)$. For this to occur, the coefficients h_{OT_i} must be equal, i.e., the heat released per mole of O_2 for each organic compound must be the same, which is usually not the case.

In the remainder of this section, we use DEB theory to obtain an expression that establishes the link between the coefficient of proportionality between the heat released and the oxygen flow and the internal energetics of the organism. In the literature this coefficient has already been used to assess the metabolic pathways in aerobic organisms. For example, Hansen et al. [21] obtained an expression that explains the difference between the mean accepted value for Thornton's coefficient and the observed proportionality coefficient by the existence of anaerobic reactions with an enthalpy change different from zero.

Eq. 4.4 and 4.9 establish a connection between the organic flows of food, j_X, and structure, j_V with the assimilation, $\dot{p}_A$, and growth powers, $\dot{p}_G$. The flow of reserve can be written as a function of the three powers using Eq. 4.2 and Eq. 4.1:

$$j_E = (\dot{p}_A - \dot{p}_M - \dot{p}_G)/\mu_E. \tag{4.29}$$

The flows j_X, j_V and j_E multiplied by M_V, can be assembled as:

$$\dot{\boldsymbol{J}}_{\mathcal{O}} = \boldsymbol{\eta}_{\mathcal{O}}\dot{\boldsymbol{p}}M_V, \tag{4.30}$$

where $\dot{\boldsymbol{p}}$ is the vector with the three powers of assimilation, growth and maintenance per C-mol of structure and $\boldsymbol{\eta}_{\mathcal{O}}$ is the matrix with the coefficients that link each organic flow with $\dot{p}_A$, $\dot{p}_M$ and $\dot{p}_G$. With Eq. 4.30 and Eq. 4.28 the coefficient of proportionality h_{OT} can be written as:

$$h_{OT} = \frac{\sum_{i=1}^{i=3} h_{OT_i}\dot{J}_{O_2}(i)\boldsymbol{\eta}_{\mathcal{O}}(i,:)\dot{\boldsymbol{p}}}{\sum_{i=1}^{i=3} \dot{J}_{O_2}(i)\boldsymbol{\eta}_{\mathcal{O}}(i,:)\dot{\boldsymbol{p}}}. \tag{4.31}$$

Eq. 4.31 establishes a link between the proportionality coefficient and the organism's internal energetic flows: assimilation, maintenance and growth. Again, if the coefficients

h_{OT_i} are the same, h_{OT} is independent of the relative amounts of energy spent in each internal process; otherwise its change can be used to assess the internal allocation of energy in the organism between assimilation, growth and maintenance.

4.4 Empirical Application

To demonstrate the practical applicability of the well-tested DEB theory to quantify thermodynamic changes in organisms we use published data on *Klebsiella aerogenes* growing in a continuous culture at different steady-states obtained from Esener et al. [14, 15]. *Klebsiella aerogenes* is growing aerobically on glycerol as the sole carbon and energy source, using ammonia as the N source, at a temperature of 35 ° C and a pH of 6.8 [14]. The products are only biomass (structure plus reserve), carbon dioxide and water [13]. The synthetic medium used by Esener et al. [13] is described by Evans et al. in [16]. More details about the experimental setup are given by Esener et al. [14].

Measurements include 26 measures of the specific CO_2 production rate (mol of CO_2 per C-mol of biomass inside the chemostat), 26 measures of the specific O_2 consumption rate, 26 measures of the yield of biomass on substrate Y_{WX} (C-mol biomass produced per C-mol of substrate consumed) and 9 measurements of the biomass composition at different steady-states [14, 15]. Each steady-state is characterized by a different throughput or dilution rate, d. The dilution rate is equal to the growth rate, j_V, because otherwise the biomass concentration in the chemostat would increase or decrease. The maximum growth rate was also measured by [14, 15].

4.4.1 DEB parameters

We used the measurements to estimate the following essential DEB parameters: $\dot{k}_E$, y_{XE}, y_{EV}, $\dot{k}_M$, g and the chemical compositions of a C-mol of structure $n_{CV} \equiv 1$, n_{HV}, n_{OV}, n_{NV} and a C-mol of reserve $n_{CE} \equiv 1$, n_{HE}, n_{OE}, n_{NE}.

The method is as follows. 1) We depart from a first guess of 13 DEB parameters. 2) For each steady-state we compute DEB variables like the functional response and the reserve density using the DEB parameters. 3) For each steady-state we calculate the predicted values of CO_2, O_2, Y_{WX} and biomass composition. 4) We compute the difference between the predicted values and the 105 measurements and make another estimation of the DEB parameters using the Newton-Raphson method. Steps 2-4 are repeated in order to minimize the sum of the squared errors. A detailed description of steps 1-3 is given below.

Estimation method

We depart from a first estimation of parameters $\dot{k}_E$, y_{XE}, y_{EV}, $\dot{k}_M$ and g and the chemical compositions of structure n_{CV}, n_{HV}, n_{OV}, n_{NV} and reserve n_{CE}, n_{HE}, n_{OE}, n_{NE}.

Eq. 4.12 is then used to compute the functional response f for each steady-state. This equation is also used to compute the maximum growth rate, r_m, that occurs when f is equal to one.

The value for m_{Em} is computed from the definition of investment ratio g given by Eq. 4.11. For each steady-state Eq. 4.5 is used to compute the reserve density m_E because $dm_E/dt = 0$.

With the reserve density m_E and the parameters n_{CV}, n_{HV}, n_{OV}, n_{NV}, n_{CE}, n_{HE}, n_{OE} and n_{NE}, the chemical composition of a C-mol of biomass is computed using:

$$n_{HW} = (n_{HV} + m_E n_{HE})/(1 + m_E), \tag{4.32}$$

$$n_{NW} = (n_{NV} + m_E n_{NE})/(1 + m_E), \tag{4.33}$$

and

$$n_{OW} = (n_{OV} + m_E n_{OE})/(1 + m_E). \tag{4.34}$$

The yield of biomass produced $j_V(1+m_E)$, on substrate consumed $f j_{Xm}$, is computed from:

$$y_{WX} = j_V(1 + m_E)/(f j_{Xm}). \tag{4.35}$$

The substrate consumption rate per mole of structure, j_X, the structure production rate per mole of structure, j_V, and the reserve production rate per mole of structure, j_E, are:

$$j_X = f j_{Xm}, \tag{4.36}$$

$$j_V = j_V, \tag{4.37}$$

$$j_E = j_V m_E. \tag{4.38}$$

The flows in Eq. 4.36, 4.37 and 4.38 are divided by $(1 + m_E)$ to be converted to flows per C-mol of biomass. Then, these flows are used together with the mass balance, Eq. 4.13, applied to each steady-state of the *Klebsiella aerogenes* culture to compute the CO_2, H_2O, O_2 and NH_3 flows. In Eq. 4.13, $\boldsymbol{n}_{\mathcal{M}}$ is the matrix with the chemical composition of minerals (CO_2, H_2O, O_2 and NH_3) and $\boldsymbol{n}_{\mathcal{O}}$ is the matrix with the chemical composition of organic compounds (X, E, V).

Parameter	**Value**	**Units**
$\dot{k}_M$	0.021	h^{-1}
$\dot{k}_E$	2.11	h^{-1}
y_{VE}	0.904	–
y_{XE}	1.345	–
g	1	–

Table 4.3: DEB parameters for *Klebsiella aerogenes*.

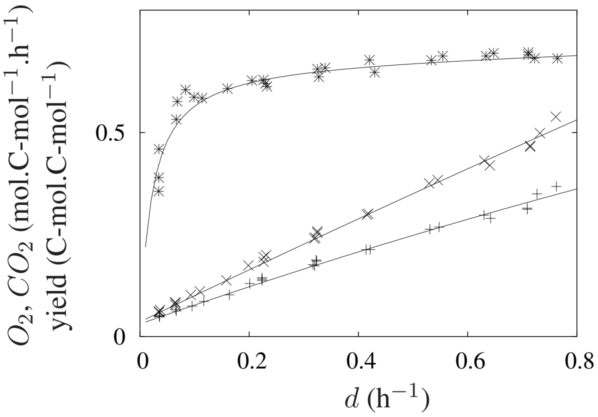

Figure 4.2: Measurements (points) and DEB model results (lines). Specific rate of consumption of O_2 $(\times)$, specific rate of production of CO_2 $(+)$ and yield $(*)$ vs. dilution rates. Units are: mol.C-mol^{-1}.h^{-1} for O_2 and CO_2 and C-mol.C-mol^{-1} for the yield.

Results

The elemental composition of structure and reserve are $CH_{1.64}O_{0.379}N_{0.198}$, and $CH_{1.66}O_{0.422}N_{0.312}$, respectively. The values obtained for the other parameters are listed in Table 4.3. The maximum growth rate measured is 1.052 h^{-1} and the value obtained with the DEB model is 1.044 h^{-1}. The comparison between the other measurements and the DEB model results is presented in Fig. 4.2 and 4.3. The root mean square error for O_2 and CO_2 are 0.0088 and 0.0086 mol.C-mol^{-1}.h^{-1} respectively and the root mean square error for Y_{WX} is 0.0249 C-mol.C-mol^{-1}. The root mean square error for n_{HW}, n_{OW} and n_{NW} are 0.009, 0.0191 and 0.0113 C-mol.C-mol^{-1} respectively. Since the fits are very good, and the DEB model obeys mass balances, we have an automatic check on the empirical mass balances, i.e., the measurements obey the mass balance. The change in the chemical composition of biomass (see Fig. 4.3) is not very significant because the chemical compositions of a C-mol of structure and a C-mol of reserve are similar with the exception of the amount of nitrogen.

The values obtained for the reserve density for each dilution rate are in Fig. 4.4.

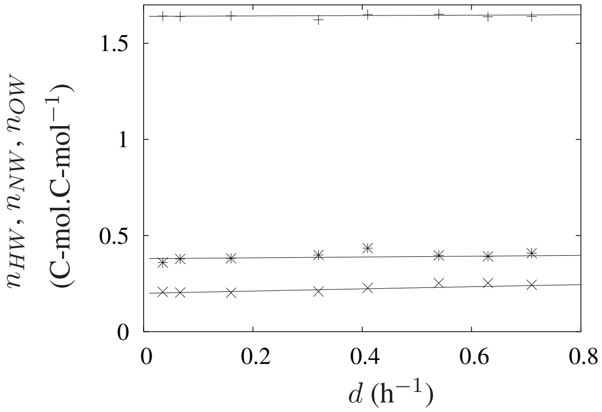

Figure 4.3: Measurements (points) and DEB model results (lines). The variable chemical composition of biomass, $n_{HW}(+)$, $n_{NW}(\times)$ and $n_{OW}(*)$ vs. dilution rates.

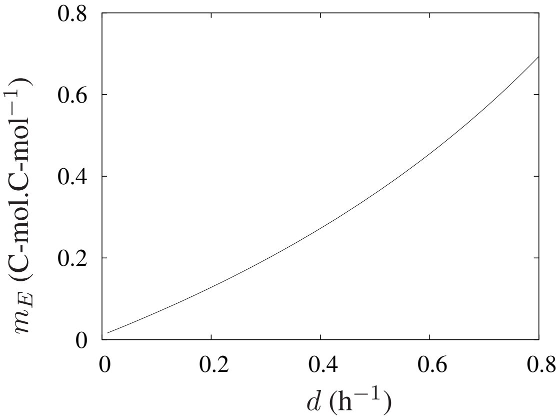

Figure 4.4: Reserve density vs. dilution rates.

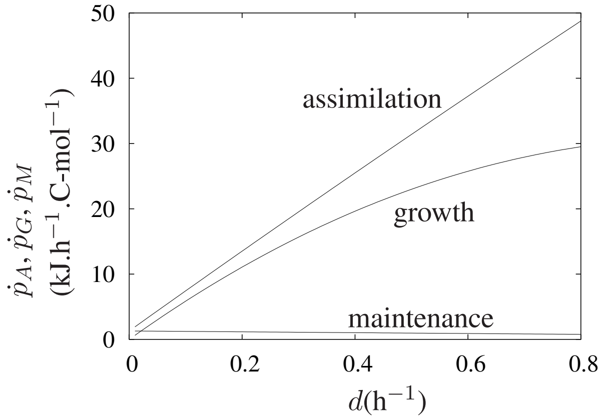

Figure 4.5: The assimilation, growth and maintenance energy flows per C-mol of biomass vs. dilution rates.

We also obtained the flows per unit of biomass of assimilation, maintenance and growth (Eq. 4.4, Eq. 4.8 and Eq. 4.9) shown in Fig. 4.5. The ratio of the assimilation flow to the food flow,

$$\dot{p}_A/\dot{p}_X = (1/y_{XE})(\mu_E/\mu_X), \tag{4.39}$$

is obtained with $\dot{p}_X = j_X \mu_X$ and Eq. 4.4. This ratio is constant because Eq. 4.39 is a function of parameters only. The assimilation flow increases with the throughput rate because the flow of food, X, also increases. Although the maintenance flow per C-mol of structure is constant because it is a function of parameters only (Eq. 4.8), the maintenance flow per C-mol of biomass decreases with the dilution rate because the reserve density increases. This occurs because it is the structure that is costly in terms of maintenance and not the reserve. The growth flow per C-mol of biomass increases with the dilution rate because it is proportional to the specific growth rate, j_V, (see Eq. 4.9) and the specific growth rate (equal to the dilution rate) increases more than the reserve density (see Fig. 4.4).

The ratio of energy spent on maintenance to energy spent on growth, given by $\dot{k}_M/r$, increases with a decreasing dilution rate, i.e., growth per C-mole of biomass becomes more expensive with decreasing dilution rate. The energetic explanation rooted in DEB theory for this behavior is: a decrease in the dilution rate translates into a lower catabolic power (defined in Fig. 5.1) and because maintenance has priority over growth a higher fraction of the catabolic power is spent on maintenance and a lower one on growth.

4.4.2 Structure and reserve specific enthalpies and entropies

The enthalpy balance

The enthalpy balance applied to the chemostat is given by Eq. 4.14. For each steady-state $\dot{\boldsymbol{J}}_{\mathcal{M}}$ and $\dot{\boldsymbol{J}}_{\mathcal{O}}$ are computed using the DEB model with the parameters estimated in the previous section. Formation enthalpies of CO_2, O_2, H_2O taken from [9] and formation enthalpy of glycerol taken from [5] were corrected for the temperature of the experiment using the specific heats at constant pressure taken from [9]. The formation enthalpy for NH_3 aq. is for 37 ° C and was taken from [20]. Values used are in Table 4.4. The enthalpies of structure and reserve are unknown but constant for all steady-states (strong homeostasis assumption). The dissipating heat depends on the steady-state and is unknown.

Eq. 4.14 is applied to different steady-states and solved for the dissipating heats and the enthalpies of structure and the reserve. This system of equations involves 2 extra unknowns. The two missing constraints were taken from Roels [30] (i.e. dissipating heats for two steady-states).

Released heats are presented in Fig. 4.6. Specific released heat ranges from -20 kJ/C-mol. to -253 kJ/C-mol (see Fig. 4.6) for increasing throughput rates. The values obtained for the released heats are of the same magnitude as the released heats presented by [31] for aerobic growth of different microorganisms on various substrates. The heat flow for each dilution rate is much higher than any of the assimilation, growth and maintenance flows (Fig. 4.6). Its magnitude is four to five times higher than the magnitude of the assimilation flow. Therefore, the energy dissipated as heat, which in an aerobic organism is a measure of the production of entropy, is a very significant energy drain.

We obtained a molar enthalpy of formation of -33 kJ/C-mol for the reserve and a molar enthalpy of formation of -107 kJ/C-mol for the structure. Thus, the formation of 1 C-mol of structure and 1 C-mol of reserve from their components at a reference state are both exothermic reactions, with the former being more exothermic. The steady-state enthalpy of the biomass, $(\overline{h}_V + \overline{h}_E m_E)/(1 + m_E)$, decreases with the dilution rate from -76 kJ/C-mol to -105 kJ/C-mol. In the literature we found no formation enthalpy values for *Klebsiella aerogenes*. Some formation enthalpy values referred in the literature are: -95.68 kJ/C-mol for *Escherichia coli* growing aerobically on succinic acid [2], -97.8 kJ/C-mol for the same microorganism [1] and -133.09 kJ/C-mol for *Saccharomyces cerevisae*.

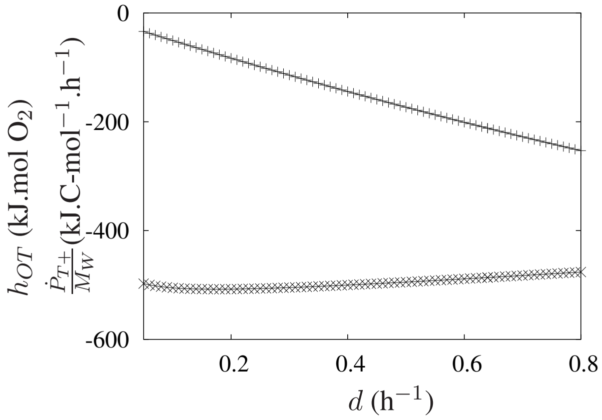

Figure 4.6: The heat production rate per C-mol of chemostat biomass per hour $(+)$ and heat production per mol of O_2 consumed $(\times)$ (Thornton's rule) vs. dilution rates. Units are: $(\times)$ in kJ.mol O_2 and $(+)$ in kJ.C-mol^{-1}.h^{-1}.

The entropy balance

The entropy balance applied to the chemostat is given by Eq. 4.16. For each steady-state $\dot{\boldsymbol{J}}_{\mathcal{M}}$ and $\dot{\boldsymbol{J}}_{\mathcal{O}}$ are computed using the DEB model with the parameters estimated in section 4.4.1. Absolute entropies were taken from Dean [9] and corrected for temperature (see Table 4.4). The entropies of structure and reserve are unknown but constant for all steady-states (strong homeostasis assumption).

Eq. 4.16 is applied to different steady-states and solved for the entropies of structure and the reserve with nonlinear regression. We obtained a molar entropy of 74.8 J/C-mol.K for the reserve and a molar entropy of of 52.0 J/C-mol.K for the structure. To test the reliability of these specific entropy values we computed the left-hand side of Eq. 4.16 for many steady-states. It is very close to zero, i.e., it is at maximum 0.04% of any other term in the equation. The first important remark is that these entropies are not null and are different from the entropies of the inputs and outputs. The steady-state entropy of the biomass, $(\overline{s}_V + \overline{s}_E m_E)/(1 + m_E)$, increases from 52.4 J/C-mol.K to 61.4 J/C-mol.K with increasing dilution rate (see Fig. 4.7). The molar biomass entropy increases with the increasing dilution rate because the reserve density increases. In the literature we found no absolute entropy values for *Klebsiella aerogenes*. Other absolute entropy values comprise: 94.4 J/C-mol.K for dried *Escherichia coli* growing on succinic acid [2] and 34.17 J/C-mol.K for *Saccharomyces cerevisae* [4].

We also compare the molar biomass entropy obtained with DEB with the entropy given by the empirical rule proposed by Battley [6] for organic substances (see Fig. 4.7). The entropy of the biomass computed by DEB theory increases more with the dilution rate and is significantly higher. However, the application of Battley's rule to dead bio-

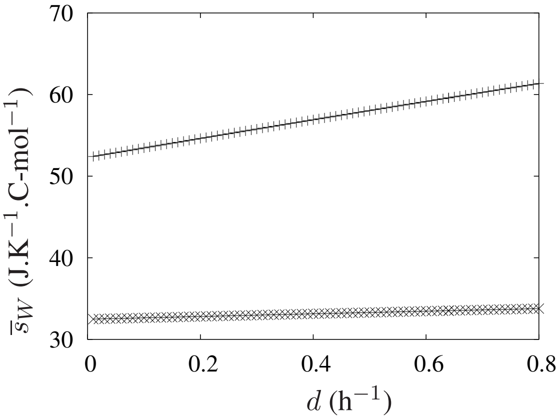

Figure 4.7: Entropy of biomass computed with DEB model $(+)$ and entropy of biomass given by Battley's rule $(\times)$ vs. dilution rates.

Formula	**State**	**Enthalpy (kJ/mol)**	**Entropy (J/mol.K)**
CO_2	g	-393.14	214.70
H_2O	l	-285.83	72.331
O_2	g	0	205.80
NH_3	aq.	-132.5	112.34
C mol glycerol	aq.[8]	-225.52	69.743

Table 4.4: Enthalpies and entropies at 35 ° C.

mass of *Saccharomyces cerevisae* [6] gave a very similar result to the entropy obtained experimentally in [4]. Therefore: (1) the entropy of dead biomass is different from the entropy of living biomass and (2) Battley's rule should not be applied for living biomass. The entropies of structure and reserve should be computed for other organisms in order to evaluate the generality of these results.

In the literature [1] the entropy of biomass has been compared to the entropy of the substrate. In our case, the biomass entropy ranges from 3.03 J/g.K to 2.69 J/g.K while the entropy of glycerol is 2.03 J/g.K. The fact that 1 gram of biomass has a higher entropy then 1 gram of substrate is in accordance with results obtained by Battley [1] for *Escherichia coli* and succinic acid. Battley argues that this result points to the fact that specific entropy is not related with complexity, otherwise, how could the lower entropy value for the substrate be explained? We disagree because we think that 1 gram is an arbitrary quantity: why not compare 1 C-mol? In that case the entropy of a C-mol of structure is lower than the entropy of a C-mol of glycerol.

4.4.3 Calorimetry

The heats released in the complete combustion of compound i per mol of consumed O_2 are: -472 kJ for the food, -485 kJ for the reserve and -447 kJ for the structure of *Klebsiella aerogenes*. These values are more or less in agreement with the values obtained theoretically by Gnaiger and Kemp [18] for other organic compounds. Although, the heats of combustion of X, E and V are similar, the net flow of food is positive while the net flows of structure and reserve are negative, suggesting that the coefficient h_{OT} is not bounded by the values of the various h_{OT_i}. This is indeed the case for the dilution rates considered, where the ratio of the heat flow to the oxygen flow varies between -476 kJ and -507 kJ per mol of O_2 consumed (see Fig. 4.6).

4.5 Conclusions

The thermodynamic analysis made in this chapter is applicable to any organism because 1) it is based on a thermodynamic formalism applicable to any open thermodynamic system and 2) uses a general model to describe the internal structure of the organism - the Dynamic Energy Budget Model.

We obtain the thermodynamic constraints for organisms with constant food availability, i.e., organisms with a constant chemical composition (DEB's weak homeostasis assumption). These constraints are that only anaerobic organisms can (1) be endothermic, (2) have a net negative import of chemical entropy while increasing their biomass and (3) have a net positive import of chemical entropy while decreasing their biomass (see Table 4.2). Apparently, anaerobic organisms have a higher thermodynamic flexibility.

We obtain Thornton's coefficient as a function of either (1) the flows of organic compounds (see Eq. 4.28), or (2) assimilation, maintenance and growth (see Eq. 4.31) using DEB theory. These relationships are useful in providing new insights into the discrepancies obtained between Thornton's constant and experimental values.

We use experimental data on the aerobic growth of *Klebsiella aerogenes* to obtain molar enthalpies and entropies for the reserve and structure. The knowledge that these properties are constant (DEB's strong homeostasis assumption) is sufficient to compute changes in the enthalpy and in the entropy of living biomass that are known to accompany changes in the reserve density. The importance of being able to compute thermodynamic properties as a function of the amount of reserves has been acknowledged in the literature, e.g., Battley [1] computes the enthalpy of a C-mol of *E. coli* under conditions that impose that ‘no storage materials are produced’. Previously, the entropy of living organisms was obtained either by (1) experimental methods or by (2) Battley’s empirical rule [4]. The use of DEB theory for these computations is better than the methods referred because (1) experimental methods are destructive and (2) Battley’ rule does not give results similar to the results we obtained. This last point suggests that the entropy of living biomass is different from the entropy of dead biomass because Battley’s rule has been validated with good results for dead biomass and organic compounds.

We introduce the mechanism of ‘dilution of entropy production by growth’ for organisms that are not in steady-state. The capacity of this mechanism to store entropy in new biomass changes with DEB’s reserve density because the molar entropy of the reserve is different from the molar entropy of the structure. We proved this for *Klebsiella aerogenes* where the entropies obtained are different from zero and the structure’s molar entropy is significantly lower than the reserve’s. Additionally, this result suggest that the reserve density concept of DEB theory is essential in discussions concerning the relationship between organization and entropy because the entropy of the organism is a function of the reserve density but the entropy of the structure, which can be related with the organization of the organism, is not.

The development of the generic thermodynamic analysis carried out in this chapter can contribute to enlighten the discussions mentioned here and others including thermodynamic measures of biological organization, the explanation of evolutionary increase in size and evolutionary strategies of energy allocation.

4.6 Appendices

4.6.1 Appendix I

In this appendix we briefly explain the notation used throughout the chapter. A list of compounds is in Tab. 4.1.

Mass of compound $*$, M_*, is measured in moles for P (product) or X (food) and in C-moles for E (reserve), V (structure) and W (biomass). The ratio $m_E \equiv M_E/M_V$ is the reserve density of the organism and m_{Em} is the maximum reserve density.

Mass flows of compound $*$, j_*, are measured in moles (or C-moles) per C-mol of structure per time. There is one exception to this rule, j_{Xm}, which is the flow of X measured in moles per C-mol of structure per unit time at the maximum ingestion rate. If mass flows are measured in moles or C-moles per unit time they are represented as

$J_* \equiv j_* M_V$.

Coefficients that relate two mass flows are y_{*1*2}. They represent the number of moles of $*1$ needed to produce one mol of $*2$. In the assimilation reactor food is converted into reserve, y_{XE}, and in the growth reactor reserve is converted into structure, y_{EV}.

Energy flows, $\dot{p}_*$, are measured in Gibbs energy per C-mol of structure per unit time. The $* = X, A, C, M, G$, stands for the process which the energy flow is associated with: X (feeding), A (assimilation), C (catabolism), M (maintenance) and G (growth). Chemical potentials convert mass flows to energy flows: μ_X converts the flow of food to $\dot{p}_X$; μ_E converts the flow of reserve that exits the assimilation reactor into $\dot{p}_A$, the flow of reserve that exits the reserve compartment into $\dot{p}_C = \dot{p}_M + \dot{p}_G$.

The energy flow $\dot{p}_X$ is associated with the adimensional functional response $f(X) \in [0, 1]$ that is equal to 1 at abundant food ($X \rightarrow \infty$) and 0 at no food availability ($X = 0$). Other DEB parameters include: the reserve turnover rate $\dot{k}_E$ and the maintenance rate coefficient $\dot{k}_M$, both parameters' dimensions are per time. The first is related with the velocity of use of the reserve and the second with the velocity of degradation of the structure. Also related with the structure there is the adimensional investment ratio g, a measure of the relative cost of building structure.

Thermodynamic properties have the usual notation: $\overline{g}_*$ is the molar Gibbs energy, $\overline{h}_*$ is the molar enthalpy, $\overline{s}_*$ is the molar entropy and $\overline{u}_*$ is the molar internal energy and μ_* is the chemical potential of compound $*$, T is the temperature, $\dot{P}_{T+}$ is the rate of heat release by the organism and $\dot{Q}_{reactions}$ is the rate of heat release by all chemical reactions inside the organism.

Vectors and matrices are in bold. The transpose of a vector is indicated by ^{T} and the inverse of a matrix is indicated by $^{-1}$. An overbar means that it is a molar quantity.

The matrix with the chemical composition is $\boldsymbol{n}$: $\boldsymbol{n}_{\mathcal{O}}$ is the matrix with the chemical composition of the organic compounds (X, P, E, V) and $\boldsymbol{n}_{\mathcal{M}}$ is the matrix with the chemical composition of the minerals (CO_2, O_2, H_2O, N_{waste}). Each entry in these matrices, n_{*1*2}, is the number of atoms of element $*1$ in compound $*2$.

4.6.2 Appendix II

The dynamics of the reserve density

$$\frac{dm_E}{dt} = f m_{Em} \dot{k}_E - \frac{\dot{p}_C}{\mu_E} - m_E \frac{1}{M_V} \frac{dM_V}{dt}, \tag{4.40}$$

is obtained by combining Eq. 4.3 with Eq. 4.4, Eq. 4.6 and $j_X = f j_{Xm}$. One of the assumptions of DEB theory is that the mobilization of reserves, i.e., the catabolic power, cannot depend on food availability, which means that it can only depend on the state variables, the reserve density, m_E, and the amount of structure, M_V. Under this assumption, the last two terms in Eq. 4.40 are a function only of m_E and M_V. So, Eq. 4.40 can be written as:

$$\frac{dm_E}{dt} = f m_{Em} \dot{k}_E - \Phi(m_E, M_V). \tag{4.41}$$

At constant food, the weak homeostasis assumption implies that the reserve density is constant $m_E = m_E^*$. Thus,

$$f m_{Em} \dot{k}_E = \Phi(m_E^*, M_V). \tag{4.42}$$

However, the weak homeostasis assumption also implies that m_E^* is dependent on food level but not on the amount of structure M_V because the organism can grow with a constant reserve density. Thus,

$$\Phi(m_E^*, M_V) = H(m_E^*), \tag{4.43}$$

because $f m_{Em} \dot{k}_E$ does not depend on M_V. The function $\Phi(m_E, M_V)$ can be generalized out of steady-state as $\Phi(m_E, M_V) = H(m_E) + (m_E^* - m_E) G(m_E, M_V)$. With this specification for $\Phi(m_E, M_V)$ eq. 4.41 becomes

$$\frac{dm_E}{dt} = f m_{Em} \dot{k}_E - H(m_E) - (m_E^* - m_E) G(m_E, M_V). \tag{4.44}$$

With Eq. 4.40 and Eq. 4.44 the catabolic flux per C-mol of structure is:

$$\begin{aligned} \dot{p}_C &= \mu_E H(m_E) + \mu_E (m_E^* - m_E) G(m_E, M_V) \\ &- \mu_E m_E \frac{1}{M_V} \frac{dM_V}{dt}. \end{aligned} \tag{4.45}$$

Additionally, $G(m_E, M_V) = 0$ because m_E^* is a function of food availability and according to DEB theory the catabolic power cannot depend on food availability. Thus,

$$\dot{p}_C = \mu_E H(m_E) - \mu_E m_E \frac{1}{M_V} \frac{dM_V}{dt}. \tag{4.46}$$

Eq. 4.46 can be written as a function of m_E, M_V and parameters using Eq. 4.10:

$$\dot{p}_C = \mu_E H(m_E) - \mu_E m_E \left(\frac{\dot{k}_E \frac{m_E}{m_{Em}} - \dot{k}_M g}{\frac{m_E}{m_{Em}} + g} \right). \tag{4.47}$$

To proceed with the derivation we need another of DEB's assumptions: the partitionability of reserves. If the organism's reserve is partitioned among different aggregates then the catabolic power that is mobilized from each aggregate must be proportional to the amount of energy embodied in it:

$$M_V \dot{p}_C(\lambda m_E, M_V, \lambda g) = \lambda M_V \dot{p}_C(m_E, M_V, g). \tag{4.48}$$

Also, the number of moles allocated to growth per mole of structure, from each aggregate, must be proportional to the amount of energy embodied in it.

The imposition that the catabolic power given by eq. 4.47 must obey eq. 4.48 implies that $\lambda H(m_E) = H(\lambda m_E)$. Therefore $H(m_E) = \gamma m_E$ and Eq. 4.46 simplifies to:

$$\dot{p}_C = \mu_E m_E \gamma - \mu_E m_E \frac{1}{M_V} \frac{dM_V}{dt}. \tag{4.49}$$

With Eq. 4.49 the reserve density dynamics given by Eq. 4.40 simplifies to:

$$\frac{dm_E}{dt} = f m_{Em} \dot{k}_E - m_E \gamma. \tag{4.50}$$

At abundant food availability, (1) the ingestion rate $j_X = j_{Xm}$ implying that $f = 1$ and (2) the steady-state reserve density is $m_E^* = m_{Em}$. With conditions (1-2) $\gamma = \dot{k}_E$ and

$$\frac{dm_E}{dt} = \dot{k}_E \left(f m_{Em} - m_E \right). \tag{4.51}$$

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Chapter 5

From empirical patterns to theory: A formal metabolic theory of life

Abstract

The diversity of life on Earth raises the question of whether it is possible to have a unique theoretical description of the quantitative aspects of the organization of metabolism. However, similarities between organisms, like von Bertalanffy's growth curves and Kleiber's law on metabolic rate, suggest that mechanisms that control the uptake and use of metabolites are common to all organisms. These and other empirical patterns widespread in biology should be the ultimate test for any metabolic theory that hopes for generality. The present study (1) collects empirical evidence on growth, stoichiometry, feeding, respiration and indirect calorimetry and synthesizes it as stylized empirical biological facts, (2) formalizes into assumptions and propositions a metabolic theory and (3) proves that these assumptions and propositions are coherent with the stylized empirical facts.

Keywords: Dynamic energy budget (DEB) theory, metabolism, Kleiber's law, von Bertalanffy growth

5.1 Introduction

In the literature, two main approaches are followed to get insights into biological phenomena: (1) the study of the complex set of biochemical reactions occurring at different rates and (2) the study of the organization of metabolism described by the mass and energy flows inside the organisms. We believe that the modeling of the biochemical networks of reactions that are taking place in the organism is useful but will not by itself lead to an understanding of life because the set of biochemical reactions occurring in the organism can be species-specific and too complex, especially for multicellular organisms. Also, the standard modeling of biochemical networks neglects the spatial structure and the complex transport and allocation processes in the organism.

In contrast, this chapter builds on the premise that the mechanisms that are responsible for the organization of metabolism are not species-specific [42]. This hope for generality is supported by (1) the universality of physics and evolution and (2) the existence of widespread biological empirical patterns among organisms.

The roadmap of this chapter is as follows. In section 5.2, the empirical patterns that characterize metabolism are synthesized and presented in a stylized manner. They are of the utmost importance because any biological non-species specific metabolic theory should predict a qualitative behavior that is compatible with these facts. We believe that such a theory has already been developed - the Dynamic Energy Budget (DEB) Theory. This theory aims to capture the quantitative aspects of the organization of metabolism at the organism level with implications for the sub- and supra-organismic levels [42, 43, 61]. In section 5.3, DEB theory is formalized for its standard model, which considers an isomorphic organism, with 1 reserve and 1 structure. This model is assumed to be appropriate for most heterotrophic unicellulars and animals. This theory is formalized in such a way that (1) the assumptions are highlighted and separated from the propositions and (2) the reasoning behind the assumptions and propositions is supported by the stylized empirical patterns or by universal laws. In DEB theory, the difference between species reduces to differences in the set of parameter values. In section 5.4, DEB theory for the relationship between parameters among different species is formalized. Section 5.5 synthesizes the links between empirical patterns, assumptions and propositions and concludes.

5.2 Empirical Patterns

In this section, we summarize the stylized empirical patterns in biology that are essential for a theoretical description of metabolic organization (see Tables 5.1, 5.2). These patterns are related with (1) the metabolic processes that are known to be widespread in organisms including feeding, growth, reproduction, maturation and maintenance; (2) the life-stages, i.e., embryo, juvenile and adult, and (3) the stoichiometry of organisms.

A theory that describes the metabolism of organisms should also be compatible with physics and evolutionary theory. The physical principles considered are: (P1) mass and energy are conserved entities; (P2) any energy conversion process leads to dissipation, i.e.,

	Stylized Facts		Empirical Evidence
Feeding	F1	During starvation, organisms are able to reproduce	animals [30, 37, 38]
	F2	During starvation, organisms are able to grow	animals [14, 19, 67, 71, 78, 89]
	F3	During starvation, organisms are able to survive for some time	animals [56, 77] bacteria [54]
Growth	G1	The growth of isomorphic organisms at abundant food is well described by the von Bertalanffy growth curve [3, 65]	animals [8, 16, 18, 70, 73, 79]
	G2	Many species do not stop growing after reproduction has started, i.e., they exhibit indeterminate growth [29, 49] Holometabolic insects are an exception	animals [36, 75]
	G3	Fetuses increase in weight proportional to cubed time [31]	animals [31, 90]
	G4	The logarithm of the von Bertalanffy growth rate of different species corrected for a common body temperature decreases almost linearly with the logarithm of the species maximum size	bacteria [42, pp.276-282] yeasts [42, pp.276-282] animals [42, pp.276-282]
	G5	The logarithm of the von Bertalanffy growth rate for organisms of the same species at different food availabilities decreases linearly with ultimate length	animals [20], [42, pp.96]
Respiration	R1	Freshly laid eggs do not use dioxygen in significant amounts	animals [6, 63, 68, 88]
	R2	The use of dioxygen increases with decreasing mass in embryos and increases with mass in juveniles and adults	animals [6, 11, 63, 66, 68, 72, 88]
	R3	The use of dioxygen scales with body weight raised to a power close to 0.75 [39]	animals [11, 66, 72]
	R4	Organisms show a transient increase in metabolic rate after ingesting food independent of their body mass - the heat increment of feeding	animals [7, 28, 35, 60, 69]

Table 5.1: Stylized facts and empirical evidence on feeding, growth and respiration.

	Stylized Facts		Empirical Evidence
Stoichiometry	S1	Well-fed organisms have a different body chemical composition than poorly-fed organisms	animals [9, 15, 30, 57] yeasts [21]
	S2	Organisms growing with constant food density converge to a constant chemical composition	animals [10, 17, 32, 50, 76]
Indirect Calorimetry	I1	Dissipating heat is a weighted sum of three mass flows: carbon dioxide, dioxygen and nitrogenous waste	animals [74]
Cells	C1	Cells in a tissue are metabolically very similar independently of the size of the organisms [58]	

Table 5.2: Stylized facts and empirical evidence on stoichiometry, indirect calorimetry and cells.

entropy production is always positive; (P3) mass and energy flows into the cell depend only on intensive properties; (P4) the morphology of an organism, i.e., the dependence of the surface area on the volume as the organism grows, controls the relative importance of processes that are proportional to surface area and processes that are proportional to volume and (P5) mass transport is proportional to surface areas because it occurs across surfaces between different environments. The evolutionary principles taken into account are: (P6) organisms have increased their control over their metabolism during evolution allowing for some adaptation to environmental changes in short periods and (P7) organisms inherit parents' characteristics in a sloppy way allowing for some adaptation to environmental changes across generations.

5.3 Theory on Metabolic Organization

The standard DEB model considers an isomorphic organism, i.e., an organism whose surface area is proportional to volume to the power $2/3$, with 1-reserve and 1-structure. Figure 5.1 summarize the standard DEB model while Table 5.3 summarizes the notation used throughout the paper.

State Variable	Dimensions	Interpretation
V	L^3	Structural volume
E	$\mathcal{E}$	Energy in reserve
E_H	$\mathcal{E}$	Energy allocated to maturation

Variable	Dimensions	Interpretation

t	T	time
e	–	Scaled reserve density
X	$\# L^{-3}$	Substrate density
L	L	Volumetric length
f	–	Scaled functional response
$\dot{p}_X$	$\mathcal{E}\,T^{-1}$	Feeding power
$\dot{p}_A$	$\mathcal{E}\,T^{-1}$	Assimilation power
$\dot{p}_C$	$\mathcal{E}\,T^{-1}$	Catabolic power
$\dot{p}_M$	$\mathcal{E}\,T^{-1}$	Volume related maintenance power
$\dot{p}_T$	$\mathcal{E}\,T^{-1}$	Surface related maintenance power
$\dot{p}_J$	$\mathcal{E}\,T^{-1}$	Maturity maintenance power
$\dot{p}_G$	$\mathcal{E}\,T^{-1}$	Growth power
$\dot{p}_R$	$\mathcal{E}\,T^{-}1$	Reproduction power

Parameter	**Dimensions**	**Interpretation**
$\{\dot{p}_{Am}\}$	$\mathcal{E}\,L^{-2}\,T^{-1}$	Surface-specific assimilation power
$[E_m]$	$\mathcal{E}\,L^{-3}$	Maximum reserve density
$[\dot{p}_M]$	$\mathcal{E}\,L^{-3}\,T^{-1}$	Volume-specific maintenance power
$\{\dot{p}_T\}$	$\mathcal{E}\,L^{-2}\,T^{-1}$	Surface-specific maintenance power
$[E_G]$	$\mathcal{E}\,L^{-3}$	Volume-specific growth costs
$\dot{v}$	$L\,T^{-1}$	Energy conductance
κ	–	Fraction of catabolic power spent on maintenance plus growth
κ_R	–	Fraction of reproduction power fixed in eggs
g	–	Investment ratio
$\dot{k}_M$	T^{-1}	Maintenance rate coefficient
$\dot{k}_J$	T^{-1}	Maturity rate coefficient
L_m	L	Maximum length
L_h	L	Heating length
E_H^b	$\mathcal{E}$	Threshold of energy investment at birth
E_H^p	$\mathcal{E}$	Threshold of energy investment at puberty
E_0	$\mathcal{E}$	Energy cost of one egg
μ_E	$\mathcal{E}\,M^{-1}$	Chemical potential

Compound specifier	**Dimensions**	**Interpretation**
X	–	Substrate (food)
E	–	Reserve
V	–	Structure
P	–	Products
M_i	–	Mineral compound i

Process specifier	**Dimensions**	**Interpretation**
A	–	Assimilation
C	–	Catabolism
M	–	Maintenance (volume related)
T	–	Maintenance (surface related)
G	–	Growth
R	–	Reproduction or Maturation

Table 5.3: List of symbols. Dimensions: – no dimension; L length; M mass; T time; $\#$ moles or C-moles; $\mathcal{E}$ energy. Symbols with (1) $\{\cdot\}$ are per unit surface area, (2) $[\cdot]$ are per unit of structural volume and (3) $\cdot$ are per unit time. Chemical compound and processes specifiers appear as subscripts to other variables.

Assumption 5.3.1 (State Variables) *The state of the organism is completely described by volume of the structure, V, the amount of energy in the reserve, E, and the amount of energy invested into maturation, E_H. The structure and the reserve are categories of generalized compounds, i.e. mixtures of a large number of compounds, that compose the biomass of the organism.*

Assumption 5.3.2 (Life-history events) *Life stage events occur when E_H exceeds certain thresholds. The initiation of feeding occurs when $E_H = E_H^b$ and the initiation of allocation to reproduction coupled to the ceasing of maturation occurs when $E_H = E_H^p$. The dynamics of E_H is*

$$\frac{dE_H}{dt} = \dot{p}_R, \qquad E_H \leq E_H^p, \tag{5.1}$$

where $\dot{p}_R$ is the power allocated to maturation if $E_H \leq E_H^p$ and the power allocated to reproduction if $E_H > E_H^p$.

Other life history events, such as cell division, metamorphosis or other stage transitions (e.g. to the pupal stage) occur also at threshold values for E_H.

The logical reasoning behind this assumption is the following. An organism that develops and produces offspring increases its complexity (or maturity) from the embryo to the adult stage. Among organisms of the same species the level of maturity at the onset of feeding behavior is the same. Also, initiation of allocation to reproduction, among organisms of the same species, occurs when they reach the same level (usually higher) of maturity. Therefore, it is reasonable to assume that the amount of energy invested

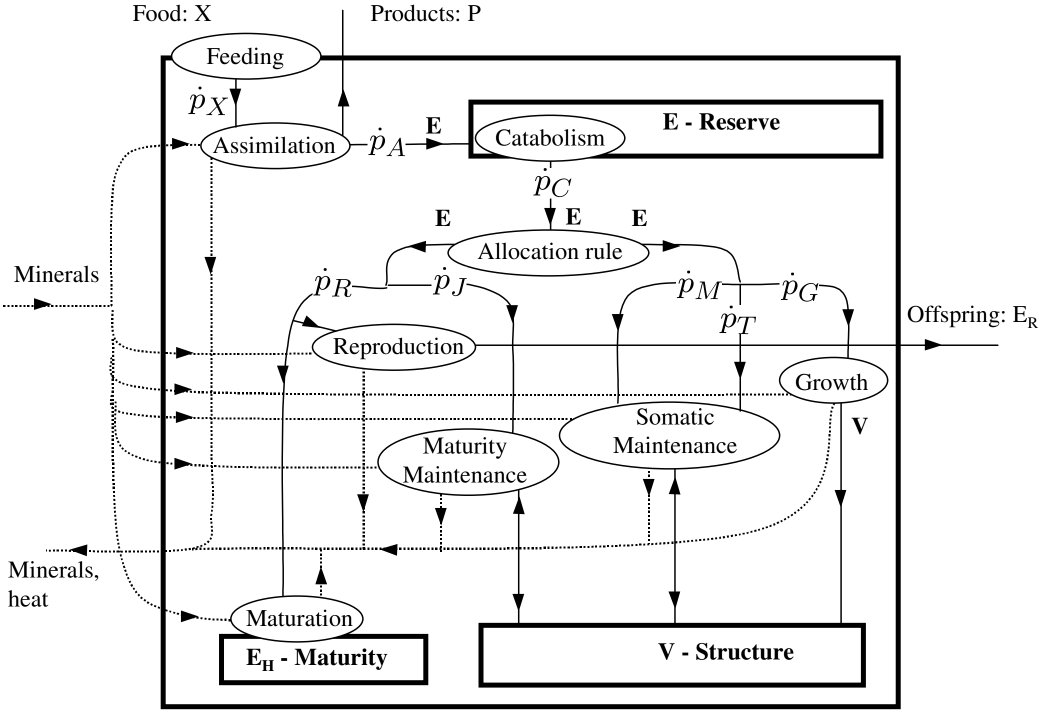

Figure 5.1: Metabolism in a DEB organism. Circles are processes; rectangles are state variables; arrows are flows of reserve (E), structure (V), minerals, food (X), products (P) or offspring (E_R).

to achieve the degrees of maturity that organisms need to start feeding or allocating to reproduction are intra-species constants.

Whenever $E_H^p > E_H^b$ multicellular organisms have three life stages. They start as an embryo or fetus that does not feed, become juveniles when the feeding behavior starts and reproduce as adults. The life history of organisms that reproduce by fission is well described by one single life-stage, the juvenile.

Assumption 5.3.3 (Strong homeostasis) *The structure, V, and the reserve, E do not change in chemical composition. The organism feeds on a resource, X, and produces products, P, also of fixed chemical compositions.*

The rationale behind strong homeostasis is (P6). Cells control the metabolism because they produce the specific enzymes needed to catalyse each chemical reaction that occurs inside the organism. However, the rate of chemical reactions also depends on the chemical composition of the surrounding environment. Thus, organisms achieve an increased control over their own metabolism (P6) by having a more stable internal chemical composition. However, empirical evidence on the variable chemical composition of the organisms, (S1), justifies the need for at least two aggregate chemical compounds, i.e., structure, V, and reserve, E.

Assumption 5.3.4 (Metabolic Processes) *Metabolism can be characterized by the following processes:*

(1) feeding - the uptake of food by the organism where $\dot{p}_X$ is the energy of the food uptake flow;

(2) assimilation - the set of reactions that transform food into reserve where $\dot{p}_A$ is the energy of this reserve flow and

(3) catabolism - the mobilization of reserve to fuel the organism activities where $\dot{p}_C$ is the energy linked with the mobilized flow. So, reserve dynamics is given by:

$$\frac{dE}{dt} = \dot{p}_A - \dot{p}_C. \tag{5.2}$$

The mobilized reserve is allocated to:

(4) growth - the increase of structure

$$\frac{dV}{dt} = \frac{\dot{p}_G}{[E_G]}, \tag{5.3}$$

where $\dot{p}_G$ is the energy of the reserve flow allocated to growth and $[E_G]$ is the specific cost of growth;

(5) somatic maintenance - the conversion of reserve into energy to fuel the set of processes

that keep the organism alive, where $\dot{p}_M$ *and* $\dot{p}_T$ *are the energy associated with the reserve flows allocated to volume and surface maintenance costs, respectively;*
(6) maturity maintenance - the conversion of reserve into energy to maintain the complexity of the structure where $\dot{p}_J$ *is the energy of the reserve flow allocated to this process and*
(7) maturation - the conversion of reserve into energy to increase the complexity of the structure where $\dot{p}_R$ *is the energy of the reserve flow allocated to this process or*
(8) reproduction - the conversion from the reserve energy of the mother into the reserve energy of the offspring where $\dot{p}_R$ *is the energy of the reserve flow allocated to this process and* $(1-\kappa_R)\dot{p}_R$ *the fraction that is dissipated. Thus,*

$$\dot{p}_C = \dot{p}_M + \dot{p}_T + \dot{p}_G + \dot{p}_J + \dot{p}_R. \tag{5.4}$$

The fraction of catabolic power allocated to somatic maintenance and growth is a general function $0 \leq \kappa(V, E) \leq 1$*, i.e.,*

$$\dot{p}_M + \dot{p}_T + \dot{p}_G = \kappa \dot{p}_C. \tag{5.5}$$

The remaining fraction of catabolic power is allocated to maturity maintenance and development or reproduction, i.e.,

$$\dot{p}_J + \dot{p}_R = (1-\kappa)\dot{p}_C. \tag{5.6}$$

All metabolic processes are a function of V*,* E *and parameters. The feeding and assimilation processes are also a function of* X*.*

Empirical evidence (R4) shows that there are processes in the organism associated with food processing only, which suggests that food goes through a set of chemical reactions that transform it into reserves - assimilation. Organisms have to spend energy on growth, maintenance and reproduction (P2). The fact that organisms are capable of spending energy on these metabolic processes in the absence of food (F1, F2, F3) suggests that the energy mobilized is obtained from the reserve and not directly from the environment. The energy mobilized for maturation is also obtained from the reserve and not from the environment because eggs do not feed but they allocate energy to maturation. The allocation of energy to growth, somatic maintenance, maturation and reproduction covers the well-known metabolic processes common to all organisms. Maturity maintenance includes maintaining regulating mechanisms and concentration gradients and defense systems. The need to allocate energy to maturity maintenance is intimately related with the second law of thermodynamics (P2) because the level of maturity, i.e., complexity of the organism, would decrease in the absence of energy spent in its maintenance. Also, the existence of an overhead cost of the reproduction process $(1-\kappa_R)\dot{p}_R$ is consistent with the dissipation principle (P2).

This assumption on metabolic organization considers that there is a flow of energy $\dot{p}_R$ that is first allocated to maturation until it ceases and then is allocated to reproduction. Assumption 5.3.4 considers that reproduction occurs immediately after maturation instead of immediately after growth because many organisms do not stop growing after reproduction has started (G2).

Assumption 5.3.5 (Metabolic Stoichiometry) *There are three different stoichiometries in the processes ocurring in the organism: assimilation, growth and dissipation. The stoichiometries of assimilation and growth are constant and given by*

$$X \longrightarrow b_A^1 P + b_A^2 E + a_A^1 M_1 + \ldots + a_A^z M_z, \tag{5.7}$$

and

$$E \longrightarrow c_G^1 V + a_G^1 M_1 + \ldots + a_G^z M_z, \tag{5.8}$$

respectively, where M_1 *to* M_z *are the mineral compounds,* b_1 *and* b_2 *are the number of C-moles of product and reserve produced per each C-mol of food processed,* a^1 *to* a^z *are the net number of moles produced of the mineral compounds* M_1 *to* M_z*. and* c^1 *is the number of C-moles of structure produced per each C-mol of reserve used.*

The stoichiometries of somatic maintenance, maturity maintenance, maturation and the stoichiometry of the dissipation of energy in reproduction are constant and all given by

$$E \longrightarrow a_1^D M_1 + \ldots + a_z^D M_z, \tag{5.9}$$

because they consist in an aggregate chemical reaction that transforms reserve plus minerals into minerals. For this reason, the sum of these powers is identified as the dissipation power

$$\dot{p}_D = \dot{p}_M + \dot{p}_J + \dot{p}_T + (1-\kappa_R)\dot{p}_R, \tag{5.10}$$

where $\kappa_R = 0$ *for the embryo and juvenile stages.*

Assumption 5.3.5 becomes a proposition under certain conditions (see Appendix 5.6.1).

Proposition 5.3.1 (Conversion Factors) *For the metabolic processes of assimilation, dissipation and growth, the conversion factors between: (1) any mass flow* $*1$ *and any energy flow* $*2$, η_{*1*2} *and (2) any mass flows* $*1$ *and* $*2$, y_{*1*2}, *are constant.*

Proof: These stoichiometric coefficients are constant because they are only dependent on the stoichiometric coefficients that are constant (Assumption 5.3.5). For example, the conversion factor between food and reserve in the assimilation process is constant because $y_{XE} = 1/b_A^2$ and the conversion factor between food and the assimilation flow is also constant because $\eta_{XA} = 1/(b_A^2\mu_E)$ and μ_E is constant (see Assumption 5.3.3). A similar reasoning can be applied to the other conversion factors. ■

Proposition 5.3.2 (Organism Stoichiometry) *The stoichiometry of the aggregated chemical transformation that describes the functioning of the organism has 3 degrees of freedom. More specifically, the flow of any compound produced or consumed in the organism is a weighted average of the flows of any three other compounds.*

Proof: The net flows (input-output) of minerals, products, heat and other compounds, at the boundary of the organism, are given by:

$$\dot{J}_{*1} = \dot{J}_{*1A} + \dot{J}_{*1D} + \dot{J}_{*1G} \tag{5.11}$$

where $*1$ stands for CO_2, O_2, $heat$, N_{waste}, H_2O and other compounds, $\dot{J}_{*1A}$, $\dot{J}_{*1G}$ and $\dot{J}_{*1D}$ are the net flows of $*1$ in the assimilation, growth and dissipation processes, respectively. Eq. 5.11 can be rewritten as:

$$\dot{J}_{*1} = \eta_{*1A}\dot{p}_A + \eta_{*1D}\dot{p}_D + \eta_{*1G}\dot{p}_G \tag{5.12}$$

where $\dot{J}_{*1A} \equiv \eta_{*1A}\dot{p}_A$, $\dot{J}_{*1G} \equiv \eta_{*1G}\dot{p}_G$ and $\dot{J}_{*1D} \equiv \eta_{*1D}\dot{p}_D$ (see definition of η_{*1*2} in Proposition 5.3.5).

To obtain $\dot{p}_A$, $\dot{p}_D$ and $\dot{p}_G$ we have to: 1) know the net flows of any 3 compounds, 2) apply Eq. 5.12 for each compound

$$\begin{bmatrix} \dot{J}_{*2} \\ \dot{J}_{*3} \\ \dot{J}_{*4} \end{bmatrix} \begin{bmatrix} \eta_{*2A} & \eta_{*2D} & \eta_{*2G} \\ \eta_{*3A} & \eta_{*3D} & \eta_{*3G} \\ \eta_{*4A} & \eta_{*4D} & \eta_{*4G} \end{bmatrix} \begin{bmatrix} \dot{p}_A \\ \dot{p}_D \\ \dot{p}_G \end{bmatrix}. \tag{5.13}$$

and 3) invert the square matrix in Eq. 5.13. This matrix is invertible if the columns are linearly independent. This independence is a fact because 1) each column is the set of conversion factors associated with each metabolic process, 2) each set is dependent on the stoichiometry of the aggregate chemical reaction that describes that process and 3) growth, dissipation and assimilation correspond to different aggregated chemical reactions.

Each power is a weighted average of the flows of 3 compounds. Thus, the flow of compound $*1$ (Eq. 5.12) can be written as a weighted average of any 3 compounds $\dot{J}_{*2}$, $\dot{J}_{*3}$ and $\dot{J}_{*4}$. ■

The method of indirect calorimetry (I1) is a particular case of Proposition 5.3.2, i.e., the flow of heat is a weighted average of carbon dioxide, dioxygen and nitrogenous waste.

Proposition 5.3.3 (Partitionability of reserve dynamics) *If the organism's reserve, E, is partitioned in the organism among categories of chemical compounds, $E_i \equiv \lambda_i E$ with $0 \leq \lambda_i \leq 1$, then 1) their relative abundances λ_i are constant, 2) the catabolic power mobilized from each category must be proportional to the amount of energy embodied in it, i.e.,*

$$\dot{p}_C(\lambda E, V) = \lambda \dot{p}_C(E, V), \tag{5.14}$$

and 3) the catabolic power mobilized to maintenance and growth, from each category, must be proportional to the amount of energy embodied in it, i.e.,

$$\kappa(\lambda E, V)\dot{p}_C(\lambda E, V) = \kappa(E, V)\lambda \dot{p}_C(E, V). \tag{5.15}$$

Proof: Each different category of chemical compounds, E_i, must represent a constant relative abundance λ_i of the aggregate reserve E, otherwise the chemical composition of reserve as a whole would change, violating Assumption 5.3.3.

The catabolic power mobilized from E_i has the chemical composition of that category of compounds. Therefore, the mobilization of the different categories of chemical compounds, E_i, must be coordinated, such that the aggregate chemical composition of the catabolic power is the same as the chemical composition of E (see the chemical composition of $\dot{p}_C$ in Assumption 5.3.4). Thus, the catabolic power mobilized from E_i must be a fraction λ_i of the aggregate catabolic power, i.e., $\dot{p}_C(E_i, V) = \lambda \dot{p}_C(E, V)$. Eq. 5.14 is obtained replacing E_i with $\lambda_i E$.

Also, the allocation to growth and maintenance of the different categories of chemical compounds, E_i, must be coordinated, such that the aggregate chemical composition of the catabolic power allocated to these metabolic processes is the same as E's (see the chemical composition of $\dot{p}_G$ and $\dot{p}_M + \dot{p}_T$ in Assumption 5.3.4). Thus, $\kappa(E_i, V)\dot{p}_C(E_i, V) = \kappa(E, V)\lambda \dot{p}_C(E, V)$. Eq. 5.15 is obtained replacing E_i with $\lambda_i E$.

■

Proposition 5.3.4 (The κ allocation rule I) *The κ function is independent of E, i.e.,*

$$\kappa(\lambda E, V) = \kappa(E, V). \tag{5.16}$$

Proof: Follows directly from Eq. 5.14 and 5.15. ■

Assumption 5.3.6 (Dependence on the Environment - Feeding) *The ingestion at abundant food is proportional to surface area, $\dot{J}_{Xm} = \{\dot{J}_{Xm}\}V^{2/3}$, where $\{\dot{J}_{Xm}\}$ is the* *maximum surface-specific feeding rate. So, the feeding power is*

$$\dot{p}_X = \{\dot{J}_{Xm}\}V^{2/3}f(X)\mu_X = \dot{J}_X\mu_X, \tag{5.17}$$

where the nondimensional functional response

$$f(X) = \frac{\dot{J}_X}{\dot{J}_{Xm}}, \tag{5.18}$$

is a monotonous increasing function of food with $0 \leq f(X) \leq 1$, $\dot{J}_X$ *is the rate of ingestion at food density* X *and* μ_X *is the chemical potential of food.*

Feeding is proportional to surface area within the same species because acquisition processes and digestion and other food processing activities depend on mass transport processes that occur through surfaces (P5).

Proposition 5.3.5 (Dependence on the Environment - Assimilation) *The assimilation power is proportional to surface area,*

$$\dot{p}_A = \{\dot{p}_{Am}\}V^{2/3}f(X), \tag{5.19}$$

where $\{\dot{p}_{Am}\} \equiv \frac{\{\dot{J}_{Xm}\}}{\eta_{XA}}$ *is the maximum surface-specific assimilation rate.*

Proof: By writing $\dot{J}_X$ in Eq. 5.17 as a function of

$$\eta_{XA} \equiv \frac{\dot{p}_A}{\dot{J}_X}, \tag{5.20}$$

it follows directly that

$$\dot{p}_A = \frac{\{\dot{J}_{Xm}\}}{\eta_{XA}}V^{2/3}f(X). \tag{5.21}$$

Proposition 5.3.5 implies that η_{XA} is constant and therefore $\{\dot{p}_{Am}\} \equiv \frac{\{\dot{J}_{Xm}\}}{\eta_{XA}}$ is also constant. ■

The energetic flows associated with the metabolic processes can be classified as supply-driven or demand-driven. This classification is sensitive to the organization level. In this paper, we classify them referring to the compartment level depicted in Fig. 5.1. Demand-driven flows are controlled by the state of the arrival compartment while supply-driven are controlled by the state of the departure compartment. Feeding and assimilation are supply-driven processes because they depend on the concentration of food in the environment, X and do not depend on E.

Assumption 5.3.7 (The κ allocation rule) *The* κ *function is independent of* V.

Note that assumption 5.3.7 together with Proposition 5.3.4 impose that κ is a constant. This assumption is supported by the following reasoning. Somatic cells take up from the blood a κ fraction of the catabolic power while ovary cells take up the rest. Since the energy flow into the ovary and somatic cells can only depend on intensive properties (P3), e.g., the blood energy content, the κ cannot depend neither on V nor on E.

Assumption 5.3.8 (Weak homeostasis) *For adults and juveniles at any constant food level,* $X = X^* > 0$, *there is a reserve density,* $[E]^*(X^*)$, *which remains constant along the growth process. Furthermore* $\lim_{X^* \to \infty} [E]^* \equiv [E_m] < \infty$, *where* $[E_m]$ *is the maximum reserve density.*

The weak homeostasis assumption is supported by the empirical evidence that growing biomass converges to a constant chemical composition as long as food density remains constant (S2). Also, empirical evidence supports the existence of a maximum size (G4, G5) (including reserve and structure) which implies that the maximum amount of energy in the reserve, E_m, is limited and the maximum reserve density, $[E_m] \equiv E_m/V$, is also limited.

Proposition 5.3.6 (Catabolic power) *Catabolic power is given by:*

$$[\dot{p}_C] = [E]\left(\dot{v}V^{-1/3} - \frac{1}{V}\frac{dV}{dt}\right). \tag{5.22}$$

where $\dot{v} \equiv \{\dot{p}_{Am}\}/[E_m]$ *is the energy conductance.*

Proof:

By the definition of reserve density, i.e., $[E] \equiv E/V$:

$$\frac{d[E]}{dt} = \frac{1}{V}\frac{dE}{dt} - \frac{[E]}{V}\frac{dV}{dt}. \tag{5.23}$$

Replacing $\frac{dE}{dt}$ by Eq. 5.2 and $\dot{p}_A$ by Eq. 5.19, Eq. 5.23 simplifies to:

$$\frac{d[E]}{dt} = \{\dot{p}_{Am}\}V^{-1/3}f(X) - [\dot{p}_C] - \frac{[E]}{V}\frac{dV}{dt}. \tag{5.24}$$

This can be written as

$$\frac{d[E]}{dt} = \{\dot{p}_{Am}\}V^{-1/3}f(X) - \Phi(V, [E]), \tag{5.25}$$

because 1) $\dot{p}_C$ is a function of E and V (see Assumption 5.3.4), 2) dV/dt is proportional to $\dot{p}_G$ (see Eq. 5.3) and 3) $\dot{p}_G$ is a function of E and V (see Assumption 5.3.4).

Assumption 5.3.8 implies that for any constant food level there is a reserve density $[E]^*$ that remains constant, i.e., $\frac{d[E]}{dt} = 0$. For $[E]^*$ Eq. 5.25 simplifies to

$$\{\dot{p}_{Am}\}V^{-1/3}f(X) = \Phi(V, [E]^*). \tag{5.26}$$

Also, Assumption 5.3.8 says that $[E^*]$ is independent of volume because it remains constant along the growth process, implying that $\Phi(V,[E]^*) = V^{-1/3}H([E]^*)$.

Function $\Phi(V,[E])$ can be generalized out of steady-state as $\Phi(V,[E]) = V^{-1/3}H([E]) + ([E^*]-[E])G(V,[E],X^*)$ imposing that $\frac{d}{dX}(([E^*]-[E])G(V,[E],X)) = 0$ because $\Phi(V,[E])$ does not depend on food. Condition $\frac{d}{dX} = 0$ implies that $G(V,[E],X) = A\frac{1}{[E^*]-[E]}$ where A is a constant, i.e., $([E^*]-[E])G(V,[E],X^*) = A$.

Using this expression, Eq. 5.24 and Eq. 5.25, the catabolic flux can be written as

$$[\dot{p}_C] = V^{-1/3}H([E]) + A - \frac{[E]}{V}\frac{dV}{dt}, \tag{5.27}$$

or

$$\dot{p}_C = V^{2/3}H([E]) + AV - [E]\frac{dV}{dt}. \tag{5.28}$$

The condition $\dot{p}_C = 0$ when the amount of reserve is null implies that 1) $A = 0$ and 2) $H([E]) = 0$ when $E = 0$. Proposition 5.3.3 on the partitionability of reserve dynamics is used to further specify $H([E])$. In the case of a fully grown adult ($dV/dt = 0$), Eq. 5.14 implies that

$$\lambda H([E]) = H(\lambda[E]). \tag{5.29}$$

Therefore $H([E]) = \dot{v}[E]$ where $\dot{v}$ is a parameter, the energy conductance, and Eq. 5.27 simplifies to:

$$[\dot{p}_C] = \dot{v}[E]V^{-1/3} - [E]\frac{1}{V}\frac{dV}{dt}. \tag{5.30}$$

■

The mobilization of reserves (catabolic power) is simultaneously a supply and demand-driven process because it depends on E and V and it is independent of the environment (food). This independence of the environment is reasonable because 1) the mobilization of reserves occurs inside the organism at a molecular level, and at that level no information concerning the external environment is available (P3), (2) it provides the organism an increased protection against environmental fluctuations and an increased control over its own metabolism (P6) and (3) the mobilization of reserves should be uncoupled from the metabolic functions of feeding and assimilation. If metabolic functions were dependent on each other then it would be much more difficult to change a particular node in the metabolic network, while avoiding complex consequences for the whole organism. Also, changes in metabolic nodes typically occur ”randomly” (blind watchmaker [12]), and if several of them are required at the same time to improve the whole organism, such improvements would be rare. The result would be that evolutionary progress would stop, while the environment continues to change.

The $[\dot{p}_C]$ decreases with the relative structural growth because the energy density decreases (dilution by growth). The $[\dot{p}_C]$ is constant for a fully grown organism at constant food level because $dV/dt = 0$ and $[E] = [E]^*$ (see Assumption 5.3.8). This means that, at constant food level, the organism has a higher degree of control over its metabolism (P6).

Proposition 5.3.7 (Energy conductance) *The energy conductance is*

$$\dot{v} = \frac{\{\dot{p}_{Am}\}}{[E_m]}. \tag{5.31}$$

Proof: With Eq. 5.30 the reserve density dynamics is:

$$\frac{d[E]}{dt} = V^{-1/3}\left(\{\dot{p}_{Am}\}f(X) - \dot{v}[E]\right). \tag{5.32}$$

At abundant food, assumption 5.3.6 defines f_X such that $f_X = 1$ and assumption 5.3.8 imposes that the reserve density $[E]$ will tend to $[E_m]$. Replacing $\frac{d[E]}{dt} = 0$, $f_X = 1$ and $[E] = [E_m]$ in Eq. 5.32 we obtain Eq. 5.31. ■

The catabolic power per unit of structural volume of a fully grown organism

$$[\dot{p}_C] = \dot{v}\frac{[E]}{V^{1/3}}, \tag{5.33}$$

is similar to a diffusion law where the flux of reserves per unit of structural volume is proportional to a reserve density gradient and to the energy conductance $\dot{v}$.

Proposition 5.3.8 (Reserve density at weak homeostasis) *The reserve density under weak homeostasis is given by:*

$$[E^*] = f(X)[E_m]. \tag{5.34}$$

Proof: At weak homeostasis $\frac{d[E]}{dt} = 0$ and Eq. 5.24 simplifies to:

$$[\dot{p}_C^*] = [E^*]\left(\dot{v}V^{-1/3}\frac{f(X^*)}{[E^*]/[E_m]} - \frac{1}{V}\frac{dV}{dt}\right). \tag{5.35}$$

Eq. 5.34 is now obtained inserting the expression for catabolic power given by Eq. 5.22. ■

Assumption 5.3.9 (Reserve and Structure - Maintenance needs) *Reserve has no maintenance needs while structure has constant (positive) maintenance needs.*

Structure maintenance costs $\dot{p}_M$ and $\dot{p}_T$ are proportional to structural volume and to surface area:

$$\dot{p}_M = [\dot{p}_M]V, \tag{5.36}$$

$$\dot{p}_T = \{\dot{p}_T\}V^{2/3}, \tag{5.37}$$

where $[\dot{p}_M]$ *and* $\{\dot{p}_T\}$ *are constant specific costs, i.e., costs per time and per unit of structural volume or area, respectively.*

Freshly laid eggs must have reserve because during the embryo stage 1) the aerobic organism uses dioxygen (R2), 2) reserve fuels all metabolic processes (Assumption 5.3.4) which implies that the embryo must have reserve and 3) there is no production of reserve during the embryo stage because the organism does not feed (Assumptions 5.3.2 and 5.3.4).

Empirical evidence (R1) shows that freshly laid eggs do not mobilize energy for metabolic processes, which means that they do not spend energy on maintenance. Thus, reserve does not pay maintenance because freshly laid eggs have reserve. However, organisms have maintenance needs because they are able to survive only for a limited time during starvation (F3). Therefore, structure has maintenance needs and freshly laid eggs are composed of reserve only. Structure constant specific maintenance needs per unit of volume and per unit of area are considered to be constant because the chemical composition of structure is constant (Assumption 5.3.3).

Structural materials require maintenance because they are continuously degraded and reconstructed. Reserves can have active metabolic functions but do not require maintenance because they are continuously used and replenished. Examples of structural maintenance costs associated with structural volume include protein turnover and with area include heating in endotherms.

Assumption 5.3.10 (Maturity - Maintenance Needs) *Maturity maintenance costs* $\dot{p}_J$ *are proportional to the cumulative amount of energy invested into maturation,*

$$\dot{p}_J = \dot{k}_J E_H, \tag{5.38}$$

where $E_H \leq E_H^p$ *and* $\dot{k}_J$ *is a positive maturity rate coefficient.*

The energy already invested in maturation, E_H, contributed to increase the amount of regulating mechanisms and gradients in the organism. Henceforth, the maturity maintenance costs, $\dot{p}_J$, increase proportional to E_H. In an adult the maturity maintenance costs are constant because maturity does not increase after the onset of reproduction.

Proposition 5.3.9 (Maturation and Reproductive Power) *The amount of energy allocated to maturation in a juvenile is*

$$\dot{p}_R = (1-\kappa)\dot{p}_C - \dot{k}_J E_H, \tag{5.39}$$

while the amount of energy allocated to reproduction in an adult is

$$\dot{p}_R = (1-\kappa)\dot{p}_C - \dot{k}_J E_H^p. \tag{5.40}$$

Proof: It follows from Eq. 5.6 and Eq. 5.38. ■

The amount of energy that an adult invests in reproduction is invested by a juvenile into maturation. If an organism is kept at a low food density such that the accumulated amount of energy invested into maturation never reaches the threshold E_H^p then the organism will never reproduce. The energy drain to maturity maintenance, $\dot{p}_J$, 1) decreases $\dot{p}_R$ (see Eq. 5.39 and Eq. 5.40) 2) and increases the duration of the juvenile stage (see Eq. 5.1).

Proposition 5.3.10 (Allocation Priorities) *Maintenance has priority over growth and maturity maintenance has priority over maturation or reproduction.*

Proof: Maintenance powers, $\dot{p}_M$, $\dot{p}_T$ and $\dot{p}_J$ given by Eq. 5.36, Eq. 5.37 and Eq. 5.38 are set by the state of the organism V, by κ and other parameters that are constant. The energy that is not needed for maintenance purposes is then allocated to growth by Eq. 5.3 and to maturation or reproduction by Eq. 5.39 or Eq. 5.40. ■

Maintenance and maturity maintenance have priority because they are demand-driven processes, i.e., they do not depend on the amount of reserve E, maintenance depends on the amount of structure V and maturity maintenance depends on the amount of energy already allocated to maturity E_H. Growth and maturation or reproduction are simultaneously demand and supply-driven processes because they depend on the amount of reserve E, the amount of structure, E, and the level of maturity E_H.

Proposition 5.3.11 (Maximum Size) *Organisms of the same species have a maximum size, V_m, i.e., organisms do not grow indefinitely.*

Proof: Somatic maintenance competes directly and has priority over growth (see Prop. 5.3.10). This is crucial because somatic maintenance increases proportional to size (see Assumption 5.3.10), which imposes a maximum size on the organism. ■

In the literature, the existence of a maximum size (including reserve and structure) is generally accepted (G4,G5) which implies that the structure also has a maximum size, V_m.

Proposition 5.3.12 (Dynamic energy budget) *The dynamic energy budget of an organism is:*

$$\frac{de}{dt} = \dot{v}L^{-1}(f(X) - e) \tag{5.41}$$

$$\frac{dL}{dt} = \frac{\dot{v}}{3}\frac{e - L_h/L_m - L/L_m}{g + e} \tag{5.42}$$

where $e \equiv [E]/[E_m]$ is the scaled reserve density, $L \equiv V^{1/3}$ is the volumetric length,

$$g \equiv \frac{[E_G]}{\kappa[E_m]} \tag{5.43}$$

is the investment ratio, i.e., the ratio of the costs of growth to the maximum amount of energy allocated to growth and maintenance, $L_h \equiv \{\dot{p}_T\}/[\dot{p}_M]$ *is the heating length and*

$$L_m \equiv \frac{\kappa\{\dot{p}_{Am}\}}{[\dot{p}_M]} = \frac{\dot{v}[E_G]}{g[\dot{p}_M]} \tag{5.44}$$

is the maximum length.

Proof: Eq. 5.41, is obtained by multiplying Eq. 5.26 by $[E_m]$ and using the definition of scaled reserve density.

Eq. 5.42 is derived by 1) replacing $\dot{p}_G$ in Eq. 5.3 by Eq. 5.5, 2) replacing $\dot{p}_C$ with Eq. 5.22 multiplied by V, 3) replacing $\dot{p}_M$ and $\dot{p}_T$ with Eq. 5.36 and Eq. 5.37, respectively, 4) rearranging to obtain

$$\frac{dV}{dt} = \frac{[E]\kappa\dot{v}V^{2/3} - [\dot{p}_M]V - \{\dot{p}_T\}V^{2/3}}{[E_G] + \kappa[E]}, \tag{5.45}$$

and 5) replacing V with L^3, $[E]$ with $e[E_m]$, $\{\dot{p}_T\}$ with $L_h[\dot{p}_M]$, $\kappa[E_m]$ with $[E_G]/g$ and $[E_G]\dot{v}/g[\dot{p}_M]$ with L_m in Eq. 5.45.

■

If an organism has no surface maintenance costs, i.e., $\dot{p}_T = 0$ and $L_h = 0$, then its ultimate length is $L_\infty = fL_m$ (see Eq. 5.42). For endotherms, surface maintenance costs are associated mainly with heating where L_h is the reduction in length due to the energy allocated to these costs. In this case the ultimate length is (see Eq. 5.42)

$$L_\infty = (fL_m - L_h)\,. \tag{5.46}$$

Proposition 5.3.13 (von Bertalanffy law) *The growth curve of an isomorphic individual at constant food availability* X^* *or at abundant food* ($f \approx 1$) *is:*

$$\frac{dL}{dt} = \dot{r}_B(L_\infty - L). \tag{5.47}$$

The von Bertalanffy growth rate $\dot{r}_B$ *is given by*

$$\dot{r}_B = \frac{\dot{v}}{3L_m}\frac{1}{g+f} = \frac{\dot{k}_M g}{3(g+f)} = \left(\frac{3}{\dot{k}_M} + \frac{3L_h}{\dot{v}} + \frac{3L_\infty}{\dot{v}}\right)^{-1}, \tag{5.48}$$

where $\dot{k}_M \equiv [\dot{p}_M]/[E_G]$ *is the maintenance rate coefficient, i.e., the ratio between the costs of maintenance and growth of structure.*

Proof: If resource density is constant, X^*, scaled reserve density is $e^* = [E^*]/[E_m] = f(X^*)$ through most of the individual's life (see Eq. 5.34). Hence, the growth curve (see Eq. 5.42) is:

$$\frac{dL}{dt} = \frac{\dot{v}}{3}\frac{f - L_h/L_m - L/L_m}{g+f}. \tag{5.49}$$

Eq. 5.47 is obtained by combining Eq. 5.49 with Eq. 5.46 and Eq. 5.48. ■

Von Bertalanffy's law (Eq. 5.47) is one of the most universal biological patterns (G1). Also, organisms of the same species at different food availabilities exhibit von Bertalanffy growth rates that are inversely proportional to ultimate length in accordance with the behavior predicted by Eq. 5.48 (G5).

This proposition provides a strong support for Assumption 5.3.7 because 1) the growth rate $\dot{r}_B$ is constant only if g is constant and 2) g is constant if κ is independent of V (Eq. 5.43).

Proposition 5.3.14 (Dioxygen Consumption) *Dioxygen consumption increases with the state of maturity E_H and with the scaled reserve density e and it can increase or decrease with structural length L.*

Proof: The dioxygen flow, given by Eq. 5.12, is

$$\dot{J}_{O2} = \eta_{O2A}\dot{p}_A + \eta_{O2D}\dot{p}_D + \eta_{O2G}\dot{p}_G. \tag{5.50}$$

This equation can be rewritten with Eq. 5.10, 5.19, 5.22, 5.36, 5.37, 5.38 and 5.39,

$$\begin{aligned}\dot{J}_{O2} &= \eta_{O2A}\{\dot{p}_{Am}\}L^2 f(X) + \\ &\quad \eta_{O2D}\left([\dot{p}_M]L^3 + \{\dot{p}_T\}L^2 + \kappa_R \dot{k}_J E_H\right) + \\ &\quad \eta_{O2D}\left((1-\kappa_R)(1-\kappa)eE_m\left(\dot{v}L^{-1} - \frac{3}{L}\frac{dL}{dt}\right)\right) + \\ &\quad \eta_{O2G}[E_G]L^2\frac{dL}{dt}.\end{aligned} \tag{5.51}$$

The change in dioxygen flow is

$$\begin{aligned}\frac{\partial \dot{J}_{O2}}{\partial E_H} &= \eta_{O2D}\kappa_R\dot{k}_J > 0, \\ \frac{\partial \dot{J}_{O2}}{\partial e} &= 3\eta_{O2D}g\left((1-\kappa_R)(1-\kappa)E_m\frac{1}{L}\frac{\partial}{\partial e}\frac{dL}{dt}\right) + \\ &\quad \eta_{O2G}[E_G]L^2\frac{\partial}{\partial e}\frac{dL}{dt} > 0, \\ \frac{\partial \dot{J}_{O2}}{\partial L} &= 2\eta_{O2A}L\{\dot{p}_{Am}\}f(X) + \eta_{O2D}\left(3[\dot{p}_M]L^2 + 2\{\dot{p}_T\}L\right) + \\ &\quad \eta_{O2D}\left((1-\kappa_R)(1-\kappa)eE_m\frac{1}{L}\left(-\frac{\dot{v}}{L} + \frac{3}{L}\frac{dL}{dt} - 3\frac{\partial}{\partial L}\frac{dL}{dt}\right)\right) + \\ &\quad 3\eta_{O2G}[E_G]\left(2L\frac{dL}{dt} + L^2\frac{\partial}{\partial L}\frac{dL}{dt}\right),\end{aligned} \tag{5.52}$$

where

$$\begin{aligned} \frac{\partial}{\partial e}\frac{dL}{dt} &= \frac{1}{3}\frac{1}{g+e}\left(\dot{v} - 3\frac{dL}{dt}\right) > 0, \\ \frac{\partial}{\partial L}\frac{dL}{dt} &= -\frac{\dot{v}}{3L_m}\frac{1}{g+e} < 0. \end{aligned} \tag{5.53}$$

The dioxygen flow 1) increases with the level of maturity E_H because $\dot{k}_J > 0$ (Assumption 5.3.10) and 2) increases with the scaled reserve density e because $\frac{\partial}{\partial e}\frac{dL}{dt}$ is always positive. The behavior of the dioxygen flow with the increase in structure L is less straightforward because 1) the first term is positive if $f > 0$, 2) the second terms is always positive because $[\dot{p}_M] > 0$ and $\{\dot{p}_T\} > 0$ (Assumption 5.3.9), 3) the third term is always negative and 4) the fourth term is positive for $L < 2/3(eL_m - L_h)$ and negative otherwise. ■

There is empirical evidence that the use of dioxygen increases with decreasing mass (or increasing structural length) in embryos (R2). This empirical fact supports assumptions 5.3.9 and 5.3.10 because to explain it with Prop. 5.3.14 we must have at least one positive maintenance cost. The reasoning is as follows: 1) $\frac{\partial \dot{j}_{O2}}{\partial e}de < 0$ - the embryo mobilizes reserves for metabolic processes but it does not feed (Eq. 5.2), i.e., $de < 0$, 2) $\frac{\partial \dot{j}_{O2}}{\partial E_H}dE_H > 0$ only if $\dot{k}_J > 0$, and 3) $\frac{\partial \dot{j}_{O2}}{\partial L} > 0$ for $L > 2/3(eL_m - L_h)$ only if $[\dot{p}_M] > 0$ or $\{\dot{p}_T\} > 0$.

Proposition 5.3.15 (Fetal Development) *If the reserves of the mother, continuously supplied to the fetus via the placenta, are considered very large, i.e., $e = \infty$ then fetal growth is given by*

$$\frac{dL}{dt} = \frac{\dot{v}}{3}. \tag{5.54}$$

Proof: Eq. 5.54 is obtained by taking the limit $e \to \infty$ in the right hand side of Eq. 5.42. ■

According to Eq. 5.54 the structural volume of the fetus is proportional to cubed time:

$$V(t) = \left(\frac{\dot{v}t}{3}\right)^3. \tag{5.55}$$

The structural volume can be converted to weight using the following auxiliary proposition.

Proposition 5.3.16 (Volume to weight) *The relationship between weight, w, and structural volume, V, is*

$$w = \left(\frac{[E]}{\mu_E} + d_V\right)V = \left(\frac{[E_m]}{\mu_E}e + d_V\right)V, \tag{5.56}$$

where d_V is the density of the structure and μ_E is the chemical potential of reserve.

Proof: The volume of the organism can be written as,

$$\frac{[E]V}{d_E\mu_E} + V, \tag{5.57}$$

where the first term is the volume of the reserve, i.e., the ratio between the reserve's energy, $[E]V$, and the reserve's energy per unit volume of reserve, $d_E\mu_E$, and d_E is the density of the reserve. The weight of the organism (Eq. 5.56) is obtained by multiplying the volume of the reserve by d_E and the volume of the structure by d_V. ■

The structural volume of the fetus can be converted to weight (Eq. 5.56) using a constant because he has access to constant (or very large) reserves. In this case, Eq. 5.55 is validated by the empirical data that suggests that fetal weight is proportional to cubed time (G3).

Proposition 5.3.17 (Intraspecific Kleiber's Law) *The metabolic rate measured by the dioxygen consumption,* $\dot{J}_{O_2}$*, of fasting animals, is proportional to* w^α *with* $\alpha \in [0.66, 1]$*. If animals have the same reserve density* e *then the proportionality constant is the same.*

Proof: For organisms kept under fasting conditions, dioxygen is consumed in growth, reproduction or maturation and maintenance, i.e.,

$$\dot{J}_{O_2} = \eta_{OD}\dot{p}_M + \eta_{OD}\dot{p}_J + \eta_{OD}\dot{p}_T + (1-\kappa_R)\eta_{OD}\dot{p}_R + \eta_{OG}\dot{p}_G, \tag{5.58}$$

where η_{OD} and η_{OG} are constant (Prop. 5.3.1).

Eq. 5.58 can be simplified to:

$$\dot{J}_{O_2} = \eta_{OD}\frac{1-\kappa_R+\kappa_R\kappa}{\kappa}(\dot{p}_M + \dot{p}_T + \dot{p}_G) + \eta_{OD}\kappa_R\dot{p}_J \tag{5.59}$$

by first inserting the expression for $\dot{p}_R$ given by Eq. 5.6 and then replacing $\dot{p}_C$ with Eq. 5.5.

The somatic and maturity maintenance powers are given by Eq. 5.36, 5.37 and 5.38 and the growth power,

$$\dot{p}_G = [E_G]\dot{v}\frac{(e - L_h/L_m)V^{2/3} - V/L_m}{g+e}, \tag{5.60}$$

is obtained by combining Eq. 5.3 with Eq. 5.42. The powers $\dot{p}_M$ and $\dot{p}_J$ are proportional to V while $\dot{p}_T$ is proportional to $V^{2/3}$ and $\dot{p}_G$ is a linear combination of $V^{2/3}$ and V. The dioxygen consumption must be approximately proportional to V^α with $\alpha \in [2/3, 1]$ because it is a linear combination of $V^{2/3}$ and V (see Appendix 5.6.2). If the animals of the same species have a similar reserve density then the proportionality constant between $\dot{J}_{O_2}$ and w^α is the same (see Eq. 5.56). ■

Empirical evidence on Kleiber's law is amply available in the literature (R3). However, if organisms of the same species do not have similar reserve densities then the available data in the literature is harder to evaluate because respiration is typically linked to body weight, which has contributions from both reserve and structure. Differences in the values of α in Kleiber's law within the same species are due to differences in the allocation of energy to growth and surface related maintenance costs.

5.4 Theory on Parameter Values

In DEB theory, the set of parameter values is individual-specific. Individuals differ in parameter values and selection leads to evolution characterized by a change in the (mean) value of these parameters (P7). The differences between species are just an evolutionary amplification of the differences between individuals, i.e., they are reduced to differences in the mean value of DEB parameters. In this section, the theory for the covariation of (mean) parameter values among species is presented.

Assumption 5.4.1 (Primary molecular based parameters) *Molecular based parameters are related to molecular processes and, for related species, are similar and independent of the ultimate size of the organism (see Tab. 5.4). These parameters include:* $[E_G]$, $[\dot{p}_M]$, $\{\dot{p}_T\}$, $\dot{k}_J$, κ, κ_R, $\dot{v}$, $[E_H^b] = \frac{E_H^b}{V_m}$ *and* $[E_H^p] = \frac{E_H^p}{V_m}$.

Parameters that characterize molecular based processes (see Tab. 5.4) are considered to be identical for related species because cells are very similar independently of the size of the organism (C1). Therefore cells of about equal size have similar growth, maintenance and maturation costs, i.e., $[E_G]$, $[\dot{p}_M]$, $\{\dot{p}_T\}$, $\dot{k}_J$, κ_R, $[E_H^b]$ and $[E_H^p]$ are equal for related species. The partitioning of energy mobilized from reserves is done at the level of the somatic and reproductive cells and therefore κ is also a molecular based process. Kooijman and Troost [48] present a possible molecular mechanism that makes clear that $\dot{v}$ is a molecular based parameter. A simpler but less precise argument to justify this is presented next. Two fully grown organisms with the same V and the same $[E]$, that belong to different but related species with different maximum lengths, have similar metabolic needs. Therefore they must have a similar rate of mobilization of reserves. This occurs if $\dot{v}$ is the same because the mobilization of reserves is proportional to $\dot{v}$ (see Eq. 5.22).

Proposition 5.4.1 (Secondary molecular based parameters) *The heating length* L_h *is similar between related species and independent of the ultimate size of the organism.*

Molecular Based Parameters	Physical Design Parameters
$\kappa^A = \kappa$	$\{\dot{p}_{Am}^A\} = \{\dot{p}_{Am}\}z$
$\dot{v}^A = \dot{v}$	$g = zg^A$
$\kappa_R^A = \kappa_R$	
$\dot{k}_J^A = \dot{k}_J$	
$[E_G^A] = [E_G]$	$[E_m^A] = [E_m]z$
$[\dot{p}_M^A] = [\dot{p}_M]$	
$\{\dot{p}_T^A\} = \{\dot{p}_T\}$	
$[E_b^{H,A}] = [E_b^H]$	$E_b^{H,A} = E_b^H$
$[E_p^{H,A}] = [E_p^H]$	$E_p^{H,A} = E_p^H$
$L_h^A = L_h$	

Table 5.4: Body Scaling Relations between different species with different maximum body sizes of L_m and L_m^A where $z = \frac{L_m^A}{L_m}$.

Proof: The heating length L_h is independent of the size of the organism because both $\{\dot{p}_T\}$ and $[\dot{p}_M]$ are molecular based parameters and $L_h = \frac{\{\dot{p}_T\}}{[\dot{p}_M]}$. ■

Proposition 5.4.2 (Physical design parameters) *Physical design parameters are proportional to the maximum length of the organism, L_m (see Tab. 5.4). These parameters include: $\{\dot{p}_{Am}\}$, $[E_m]$, E_H^p, E_H^b and g.*

Proof: Suppose that a reference species and species A are related and that $z = \frac{L_m^A}{L_m}$ is the ratio of maximum lengths.

The surface specific assimilation rate is proportional to maximum length (see Eq. 5.44) because the molecular based parameters are equal for both species, $\kappa = \kappa^A$ and $[\dot{p}_M] = [\dot{p}_M^A]$:

$$z = \frac{L_m^A}{L_m} = \frac{\{\dot{p}_{Am}^A\}}{\{\dot{p}_{Am}\}}. \tag{5.61}$$

The maximum reserve density $[E_m]$ is proportional to maximum length, i.e., $[E_m^A] = z[E_m]$ because $\dot{v} = \dot{v}^A$ and $\{\dot{p}_{Am}^A\} = z\{\dot{p}_{Am}\}$ (see Eq. 5.31).

The energy investment threshold at puberty E_p^H is proportional to maximum length, i.e., $E_p^{H,A} = z^3 E_p^H$ because $[E_p^{H,A}] = [E_p^H]$. Also, the energy investment threshold at birth E_b^H is proportional to maximum length, i.e., $E_b^{H,A} = z^3 E_b^H$ because $[E_b^{H,A}] = [E_b^H]$.

The investment ratio g is proportional to maximum length, i.e., $g = zg^A$ because $[E_G] = [E_G]_A$, $\kappa = \kappa^A$ and $[E_m^A] = z[E_m]$ (see Eq. 5.43).

■

Proposition 5.4.3 (von Bertalanffy growth rate) *The von Bertalanffy growth rate for species A at abundant food is:*

$$\log \dot{r}_B^A = \log \frac{\dot{v}}{3} - \log(gL_m + L_m^A). \tag{5.62}$$

where all parameters with the exception of L_m^A *are for a reference species.*

Proof: At abundant food, i.e., $f = 1$, the von Bertalanffy growth rate (Eq. 5.48) for species A is:

$$\dot{r}_B^A = \frac{\dot{v}^A}{3L_m^A} \frac{1}{g^A + 1}. \tag{5.63}$$

Eq. 5.62 is obtained by (1) rewriting the DEB parameters of species A as a function of the DEB parameters of the reference species using Tab. 5.4 and then (2) applying logarithms. ■

This proposition on the inter-species comparison of Von Bertalanffy growth rate corrected for a common body temperature is supported by empirical data (G5)(for a comparison between empirical data and DEB model predictions see [42, Fig. 8.3]).

Proposition 5.4.4 (Interspecific Kleiber's Law) *The metabolic rate measured by the dioxygen consumption,* $\dot{J}_{O_2}$*, of fasting fully grown adult animals, that belong to species with different maximum body sizes, is proportional to* w^α *with* $\alpha \in [0.5, 1]$.

Proof: For fully grown organisms kept under fasting conditions, the dioxygen is consumed in reproduction and in somatic and maturity maintenance, i.e.,

$$\dot{J}_{O_2} = \eta_{OD}(\dot{p}_M + \dot{p}_J + \dot{p}_T + (1 - \kappa_R)\dot{p}_R), \tag{5.64}$$

where η_{OD} is constant (Prop. 5.3.1).

Eq. 5.64 can be simplified to Eq. 5.59 where $\dot{p}_G = 0$ by first inserting the expression for $\dot{p}_R$ given by Eq. 5.6 and then replacing $\dot{p}_C$ with Eq. 5.5.

The somatic and maturity maintenance powers can be written for fully grown adults ($l = 1$ and $E_H = E_H^p$):

$$\dot{p}_M = [\dot{p}_M]V_m^A, \tag{5.65}$$

$$\dot{p}_T = \{\dot{p}_T\}V_m^{A\,2/3}, \tag{5.66}$$

$$\dot{p}_J = \dot{k}_J[E_H^p]V_m^A, \tag{5.67}$$

where all parameters are for the reference species with the exception of the maximum body size of the species being considered V_m^A. Eq. 5.65 to 5.67 were obtained from Eq. 5.36, 5.37 and 5.38 respectively, by first replacing body size V with V_m because

$l = 1$ and then rewriting DEB parameters of the species being considered, species A, as a function of the DEB parameters of a reference species using Tab. 5.4 with the exception of the maximum body size, V_m^A.

The powers $\dot{p}_M$ and $\dot{p}_J$ are proportional to maximum body size volume V_m^A while $\dot{p}_T$ is proportional to ${V_m^A}^{2/3}$. The dioxygen consumption must be approximately proportional to ${V_m^A}^{\alpha}$ with $\alpha \in [2/3, 1]$ because it is a linear combination of ${V_m^A}^{2/3}$ and V_m^A.

The relationship between the weight and the volume of the species considered,

$$w = \frac{[E_m]e}{\mu_E V_m^{1/3}} {V_m^A}^{4/3} + d_V V_m^A, \tag{5.68}$$

is obtained from Eq. 5.56 by replacing body size V with V_m, energy density $[E]$ with $[E_m]e$ and rewriting the parameters of species A as a function of the parameters of a reference species with the exception of V_m^A. Thus, (1) the mass is approximately proportional to V_m^β with $\beta \in [1, 4/3]$ and (2) the dioxygen consumption is approximately proportional to $w^{\alpha/\beta}$ with $\alpha/\beta \in [0.5, 1]$.

■

The proposition obtained that the power in Kleiber's law can be in the interval $[0.5, 1]$ is more adequate that a unique value of $3/4$. This is supported by Dodds et al.'s [13] reanalyses of datasets. These authors tested whether the power is $3/4$ or $2/3$ finding little evidence for rejecting the power $2/3$. Also, Vidal and Whitledge [87] found powers of 0.72 and 0.85 for crustaceans and Phillipson [64] found values of 0.66 for unicellulars and 0.88 for ectotherms.

According to Proposition 5.4.4, the proportionality between dioxygen production and weight, in interspecies comparisons of fully grown adults, has a variable power because of a variable allocation to surface related maintenance costs, e.g., heating, $\dot{p}_T$.

5.5 Conclusions

Syntheses of DEB theory and discussions of the underlying concepts have already been presented in the literature [61, 43, 82, 83]. However, in this chapter, we formalize DEB in a set of assumptions and propositions proving 1) that DEB is a theory for the metabolic organization of organisms fully supported by the empirical biological patterns and the universal laws of physics and evolution and 2) a theory for metabolic organization can be as formal as physics.

This theory considers that body mass is partitioned into structure and reserves - two state variables of the model - which is supported by empirical evidence that organisms can have a variable stoichiometry (S1). Reserve does not require maintenance because it is passively continuously used and replenished while structure requires maintenance because it is actively continuously degraded and reconstructed. These two metabolic facts are supported by the fact that freshly laid eggs do not use dioxygen in significant amounts and that the use of dioxygen increases with decreasing mass in the embryo and with increasing mass in the juvenile and adult (R1, R2).

Feeding is considered to be proportional to surface area within a species because transport occurs across surfaces (P5). In the organism (1) food is transformed into reserve and (2) reserve is mobilized to fuel growth, maturation, maintenance and reproduction. This internal organization is suggested by the empirical evidence on the heat increment of feeding (R4) and by the fact that starving organisms survive, grow and reproduce (F1-F3).

Additionally to the processes of growth, maturation, maintenance and reproduction, organisms also allocate energy to maturity maintenance, which is imposed by the need to spend energy to keep the organism far away from equilibrium (P2). The assumption on metabolic organization considers that the flow of energy allocated to reproduction, in an adult, was allocated to maturation in a juvenile instead of being allocated to growth because many organisms do not stop growing after reproduction has started (G2).

The amount of energy invested into maturation is the third state variable. It controls life history events such as the initiation of feeding and the initiation of reproduction coupled to the ceasing of maturation. Whenever reproduction starts after the initiation of feeding the three life stages of multicellular organisms are: embryo or fetus, juveniles and adults.

The metabolic organization is further restricted by the κ rule and the weak homeostasis assumption. The κ rule imposes 1) that the allocations of energy to reproduction and growth do not compete with each other which is suggested by the laws of mass and energy transfer (P3); 2) that the energy allocation to growth competes with the energy allocation to somatic maintenance imposing a maximum size within a species (G4, G5) and 3) that the growth rate at constant food availability is constant - Von Bertalanffy law (G1, G5). The weak homeostasis assumption imposes that organisms tend to a constant chemical composition in an environment with constant food availability; this is supported by empirical evidence on a constant stoichiometry under certain conditions (S2) and motivated by evolutionary theory (P6).

The propositions obtained explain the following empirical findings: (1) the method of indirect calorimetry (I1), (2) von Bertalanffy growth curves, (3) the variation of von Bertalanffy growth rates within (G5) and across species (G4), (4) Kleiber's law on metabolic rate (R3) and (5) the pattern of fetal growth (G3).

These assumptions and propositions are at the core of DEB theory. This theory has already been tested for many organisms including bacteria [4, 5, 45, 80], crustaceans [41], collemboles [34], appendicularians [42], rotifiers [2], yeasts [21], molluscs [22, 25, 26, 27, 84], unicellular alga [42], lichens [42], nematodes [1, 23, 24, 33], fishes [85, 86] and birds and mammals [42, 90].

In this chapter, we focus on the standard DEB model for isomorphs with one reserve and one structure. They are ideal to explain the concepts, and demonstrate the importance surface area - volume interactions, which is an important organizing principle, in combination with mass and energy conservation. However, from an evolutionary perspective they represent an advanced state that evolved from systems with more reserves and, therefore, less homeostatic control. The evolution of metabolism as a dynamic system is discussed in [48]. Extensions to the standard DEB model that were not discussed in this chapter include: (1) shape corrections for the surface area of organisms that do not behave as isomorphs but deviate from this in predictable ways [42, pp.26-29]; (2) the dependence of physiological rates on body temperature [42]; (3) the inclusion of more reserves (for organisms feeding on simple substrates) and more structures (plants) [42, pp.168]; (4) an aging model that explains the phenomenological Weibull [42, pp.141] and the Gompertz laws [55]; (5) shrinking whenever the catabolic power mobilized from reserves is not enough to pay maintenance [81] and (6) implications for cellular levels [47], trophic chains and population dynamics [40, 52, 51, 53, 59] and ecosystem dynamics [44, 46, 62].

This chapter contributes to a research agenda on a non-species specific metabolic theory by (1) proposing a set of stylized empirical patterns that are the ultimate test to any metabolic theory and (2) using these facts to establish a set of assumptions and obtaining the propositions that follow. The validity of each assumption and empirical fact considered can be independently discussed leading to a wider consensus in the metabolic field.

5.6 Appendices

5.6.1 Appendix I

Proposition 5.6.1 (Metabolic Stoichiometry) *If the number of chemical elements that participate in the assimilation process is more than or equal to* $z+2$ *then the stoichiometry of assimilation is constant. If the number of chemical elements that participate in the growth process is more than or equal to* $z+1$ *then the stoichiometry of growth is constant.*

If the number of chemical elements that participate in the dissipation process is more than or equal to z *then the stoichiometry of dissipation is constant.*

Proof: The $z + 2$ stoichiometric coefficients a_1 to a_z, b_1 and b_2 of the assimilation process (Eq. 5.7) are completely determined if we have at least $z + 2$ chemical elements because each chemical element must obey a mass balance. The same reasoning applies to the growth and dissipation processes. ■

This proof assumes that the chemical composition of food, feces, reserve and structure are constant (Assumption 5.3.3). Otherwise, the stoichiometry of the metabolic processes referred would have higher degrees of freedom.

5.6.2 Appendix II

Suppose that we want make the following approximation for a polynomial

$$ax^{2/3} + bx \approx cx^{\alpha}, \tag{5.69}$$

in a given interval $[x^-, x^+]$, where $a > 0$, $b > 0$ and $c > 0$ are constants. In this case, we will choose α and c such that the total approximation error $\int_{x^-}^{x^+} (y(x,\alpha)x^{\alpha} - cx^{\alpha})^2 dx$ is as small as possible.

To minimize the total error we impose that 1) there is a point x^* within the interval $[x^-, x^+]$ such that the error is null, i.e.,

$$c = ax^{*2/3-\alpha} + bx^{*1-\alpha}, \tag{5.70}$$

and that 2) at x^* the change with x is null, i.e.,

$$\left(\frac{\partial y(x,\alpha)x^{\alpha} - cx^{\alpha}}{\partial x}\right)_{x=x^*} = (2/3 - \alpha)\, ax^{-1/3} + (1-\alpha)b = 0, \tag{5.71}$$

or that

$$\alpha = 1 - \frac{1}{3}\frac{ax^{-1/3}}{ax^{-1/3} + b}. \tag{5.72}$$

The optimal value for α is within the interval $[2/3, 1]$ because $0 < \frac{ax^{-1/3}}{ax^{-1/3}+b} < 1$. The optimal value for c is within the interval given by Eq. 5.70 for $\alpha \in [2/3, 1]$ and $x^* \in [x^-, x^+]$.

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Abstract

In this dissertation, we use thermodynamic theory to analyse biological and economic systems, according to two methodological approaches. The substantive integration is a methodological approach that consists of making two different fields physically compatible either by reformulating current theories or by building up new theory. Thermodynamics must be compatible with the theories that explain and describe economic and biological systems because thermodynamic laws impose constraints on mass, energy and entropy flows. A formal analogy is a methodological approach that consists of the development of an isomorphism between the mathematical formalisms of different fields. Thermodynamics has a solid mathematical formal structure that describes equilibrium, non-equilibrium and self-organized systems that should be common to thermodynamics, biological and economic systems. In this dissertation, we concentrate on the substantive integration between non-equilibrium thermodynamics and biological systems described by the Dynamic Energy Budget (DEB) theory and on the formal analogy between equilibrium thermodynamics and economic systems described by the neoclassical economic theory. In this dissertation, we also build a more systematic description of DEB theory as an intermediate step to a future substantive integration between thermodynamics, economics and biology.

Keywords: Thermodynamics, Formal Analogy, Substantive Integration, Dynamic Energy Budget Theory and Neoclassical Microeconomics

Samenvatting

In dit proefschrift gebruiken we thermodynamische theorie om biologische en economische systemen te analyseren, volgens twee methodologische benaderingen. De inhoudelijke integratie is een methodologische benadering die twee verschillende terreinen natuurkundig met elkaar vereenigbaar maakt door bestaande theoriën te herformuleren, of nieuwe op te zetten. De thermodynamika moet vereenigbaar zijn met theoriën die economische en biologische systemen beschrijven en verklaren, omdat haar wetmatigheden randvoorwaarden opleggen op massa, energie en entropie stromen. Een formele analogie is een methodologische benadering die bestaat uit de ontwikkeling van een gelijkvormig wiskundig formalisme voor verschillende terreinen. De thermodynamika heeft een solide formele struktuur die systemen beschrijft die wel of niet in evenwicht verkeren of zelf-organiserend zijn en kunnen worden toegepast in de thermodynamika, de biologie en de economie. In dit proefschrift concentreren we ons op een inhoudelijke integratie tussen niet-evenwichts thermodynamika en biologische systemen zoals die vastgelegd worden door de Dynamische Energie Budget (DEB) theorie en op de formele analogie tussen evenwichts-thermodynamika en economische systemen die beschreven worden door de nieuw-klassieke economische theorie. We zetten ook een meer systematische specificatie van de DEB theorie op als tussenstap voor een toekomstige inhoudelijke integratie tussen thermodynamika, economie en biologie.

Resumo

Nesta tese, usamos a teoria termodinâmica para analisar os sistemas biológicos e económicos através de duas metodologias. A integração substantiva é a metodologia que consiste em tornar dois campos do conhecimento compatíveis, através da reformulação das teorias existentes ou através da construção de nova teoria. A termodinâmica tem que ser compatível com as teorias que explicam e descrevem os sistemas económicos e biológicos porque as leis termodinâmicas impõe restrições nos fluxos de massa, energia e entropia. A analogia formal é a metodologia que consiste no desenvolvimento de um isomorfismo entre os formalismos matemáticos de diferentes áreas. A termodinâmica tem uma estrutura matemática formal que descreve os sistemas em equilíbrio, não-equilíbrio e auto-organizados que deve ser comum aos sistemas termodinâmicos, biológicos e económicos. Nesta dissertação, é feita a integração substantiva entre a termodinâmica de não equilíbrio e os sistemas biológicos descritos pela teoria 'Dynamic Energy Budget' (DEB) e é construída uma analogia formal entre a termodinâmica de equilíbrio e os sistemas económicos descritos pela teoria económica neoclássica. Nesta dissertação, construímos também uma descrição mais sistemática da teoria DEB como um passo intermédio para uma futura integração substantiva entre a termodinâmica, a economia e a biologia.

Palavras Chave: Termodinâmica, Analogia Formal, Integração Substantiva, Teoria ‘Dynamic Energy Budget’ e Microeconomia Neoclássica

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