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Is spatially integrated entropy production useful to predict the dynamics of ecosystems?

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ABSTRACT

Production of entropy by macroscopic systems in far from equilibrium as estimated from the spatial integration of the entropy production density have been considered as an important concept that could help understand and predict the evolution of open systems. In this study we have used an extensive dataset of energy fluxes recorded in Ameriflux sites to compute the entropy production across different climates and ecosystems in order to analyze whether there are clear patterns showing a higher entropy production in more vegetated sites or in more developed stages. The entropy budget has been defined over a conceptualized system defined by the Earth's Critical Zone. Based on previous studies we have recognized four different formulations for the estimation of entropy production in macroscopic systems: (i) a total entropy production that accounts for all the energy fluxes including radiation fluxes, (ii) an entropy production that includes only those fluxes of energy absorbed within the open system, (iii) an entropy production that includes only living components and accounts for biochemical energy absorbed during photosynthesis and its further dissipation in the form of heat via respiration, and (iv) an entropy production that includes only incoming and outgoing heat fluxes into the open system that occurs at different temperatures. We quantified these entropy productions at different sites and stages of ecosystem development using available information recorded in 36 Ameriflux sites. We observed rather different magnitudes and patterns in all these formulations of the entropy production. Therefore, these formulations cannot be compared or considered as the same concept as has been done previously because they represent different scales and processes. In addition, we did not find a clear evidence of a maximum entropy production in more vegetated sites and at more mature stages of development, for any of these four entropy production formulations. These results suggest that hypotheses based on a maximum entropy production estimated from spatial integration over macroscopic systems in far from equilibrium should not be considered as a fundamental principle to understand or predict the evolution of these systems.

1. Introduction

Since thermodynamic entropy (hereafter entropy) was proposed initially by Clausius in 1865 it has been considered as a promising concept that could lead us to the understanding of the evolution of different kinds of open systems. In particular, the production of entropy has been considered as a major concept that could provide important information of a system and predict its behavior. Today, more than two centuries after it was developed many different hypotheses have been proposed in the light of entropy production. However, none of these hypotheses have been fully proven. In particular, a major difficulty lies in the implementation of entropy related principles to areas that are dealing with macroscopic scales where different assumptions including temporal thermal equilibrium and spatial integration of entropy production are considered. In this study we analyze the production of entropy in the Earth's Critical Zone, and in order to compute the entropy production over this domain we use an extensive database of energy fluxes that allows us to compare the entropy production across different climates and at different stages of ecosystem development.

The most important hypotheses in the light of entropy production are the minimum entropy production principle (MinEnt) by Prigogine (1947) and the maximum entropy production principle (MEPP) proposed initially by Ziegler (1963, 1983). On the one hand, MinEnt suggests that systems in the linear non-equilibrium regime reach a steady state at which the entropy production from the system is constant and attains a minimum value (Kondepudi

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and Prigogine, 1998). Previous studies have questioned the validity of MinEnt (Martyushev and Seleznev, 2006; Martyushev, 2013; Jaynes, 1980; Palffy-Muhoray, 2001; Danielewicz-Ferchmin and Ferchmin, 2000; Hoover, 2002). In particular, Martyushev and Seleznev (2006) and Martyushev (2013) showed that MinEnt could be conceptualized as an special case of MEPP. On the other hand, MEPP as proposed initially by Ziegler (1963, 1983) suggests that when thermodynamic forces are preset the fluxes are such that there is a maximization of the entropy production density (Martyushev and Seleznev, 2006). It is important to keep in mind that MEPP implies a maximization of the entropy density δ defined over a fundamental spatial domain where the thermal equilibrium assumption remains valid. Different fields, including atmospheric sciences, hydrology, ecology, pedology, and geomorphology, have looked at MEPP as an alternative to predict the evolution of systems. However, these fields deal with macroscopic domains where the definition of such a fundamental scale is challenging. As a result, previous studies (Lucia, 2014; Ozawa et al., 2003; Kleidon et al., 2010) in these fields have modified the MEPP. This modified version, here we call *ModMEPP*, suggests that the evolution of open macroscopic systems in far from equilibrium is guided toward a maximum entropy production σ that is defined over the entire domain by spatial integration of the entropy production density:

$$\sigma = \int \delta \tag{1}$$

where δ is the entropy production density. This formulation involves an integration of the entropy production density over domains where the thermal equilibrium assumption is no longer valid. Therefore, some previous authors such as Martyushev (2013) claim that maximization of σ as suggested in ModMEPP may not be valid.

Although the validity of ModMEPP is still under debate, it could have a significant contribution in areas dealing with macroscopic systems. Computation of σ by spatial integration could be attained with measurements of energy fluxes and temperature performed in macroscopic domains. Different examples of macroscopic systems where such an approach has been performed include a cell (Lucia, 2014), a leaf (Aoki, 1989), an ecosystem (Aoki, 1995; Holdaway et al., 2010), the global water cycling (Porada et al., 2011; Westhoff et al., 2014), a portion of the atmosphere (Paltridge, 1975; Pauluis and Held, 2002), or even the entire planet (Aoki, 1983; Lorenz and Norman, 2002). As a result, validation of ModMEPP is more doable than MEPP. In fact, while there are still no clear methodologies to validate MEPP, many previous studies have performed validations of ModMEPP. For instance, in atmospheric sciences different studies trying to understand the exchange of heat fluxes within the atmosphere and with the ocean have found that ModMEPP is able to reproduce observed patterns (see Ozawa et al., 2003). Similarly, studies with FLUXNET towers in ecosystems found that entropy production increases in the more developed ecosystems, supporting ModMEPP (Holdaway et al., 2010). However, more recent studies in ecological networks (Meysman et al., 2010) claimed that the evolution of such systems is not always guided by a maximum production of entropy. In addition, studies performed on different atmospheric conditions show that rather different conditions and dissipations of energy could attain the same magnitude of entropy production by different mechanisms (Pauluis and Held, 2002), which indirectly disprove ModMEPP.

ModMEPP has also been proposed as a leading hypothesis to understand the evolution of terrestrial ecosystems. Previous studies have suggested a connection between life and higher production of entropy (Schneider and Kay, 1994; Ulanowicz and Hannon, 1987), and according to Kleidon (2004) the presence of vegetation in different parts of the Earth support this hypothesis. In addition, Holdaway et al. (2010) compared σ at different stages of ecosystem development and found that σ increases in the more developed ecosystems, which in turn support ModMEPP. However, some of previous studies have been supported on deductions based on expected patterns, instead of actual quantifications of σ. On the other hand, the studies that have quantified σ have analyzed few ecosystems and have used different periods throughout the year that has been selected arbitrarily. Therefore, it is important to perform a more comprehensive comparison that includes diverse ecosystems and climates. In this study we used an extensive database of energy fluxes over different climates to bring more evidence into the patterns of the entropy production σ in terrestrial ecosystems, and analyze whether these patterns support ModMEPP. The system under study is the Earth's Critical Zone (CZ), which according to NRC (2001), is defined as the *heterogeneous, near surface environment in which complex interactions involving rock, soil, water, air, and living organisms regulate the natural habitat and determine the availability of life-sustaining resources*. The definition of this system allows us to take advantage of the extensive dataset recorded in FLUXNET Towers (Ameriflux sites) to analyze the budget of entropy in different sites and at different developmental stages.

An important consideration that most studies have overlooked is the actual formulation that is implemented for the estimation of the entropy production. Previous studies have used different formulations for σ, and the outcomes from different formulations may result in different patterns. Based on previous studies we recognized the following formulations that have been considered for the estimation of σ: (i) some approaches include all the sources of energy that reach the system under analysis, including incoming radiation, heat, and chemical energy, (ii) other approaches neglect radiation fluxes because they claim most of radiation is dissipated instantaneously by the surface and include only the energy fluxes in the form of heat and chemical energy, and (iii) yet other approaches consider that the most interesting component to analyze is the fluxes with the highest levels of specific exergy and include only chemical energy (neglecting heat) that is absorbed by the system under analysis. These different formulations for the estimation of σ are defined on different scales and include different processes. Thus, it is unclear whether all of them lead to similar patterns, and whether all of them support ModMEPP.

The goals of this study are: (i) to quantify the production of entropy σ in the CZ for the formulations of entropy production that have been discussed above, (ii) to analyze whether computed σ from these formulations have the same patterns across climates and stages of ecosystem development, and (iii) to analyze whether these patterns support ModMEPP for terrestrial ecosystems.

2. Theory

2.1. Formulations for entropy production

Previous studies have implemented different formulations for the computation of entropy. In this section we define these formulations and explain how these approaches are applied to the CZ.

2.1.1. Total entropy production σ

Previous studies (Aoki, 1987; Holdaway et al., 2010) have conceptualized the production of entropy by considering all the fluxes that reach the domain under analysis. As a result, the production of entropy in these approaches is quantified by including the