A blueprint for thermodynamically consistent box models and a test bed for thermodynamic optimality principles

Stan Schymanski<sup>1</sup> and Martijn Westhoff<sup>2</sup>
<sup>1</sup>Catchment and Eco-Hydrology, ERIN, Luxembourg Institute of Science and Technology, Esch-sur-Alzette, Luxembourg (stanislaus.schymanski@list.lu)
<sup>2</sup>Faculty of Science, Earth and Climate, Vrije Universiteit Amsterdam, Amsterdam, The Netherlands (m.c.westhoff@vu.nl)

Thermodynamic optimality principles, such as maximum entropy production or maximum power extraction, hold a great promise to help explain self-organisation of various compartments of planet Earth, including the climate system, catchments and ecosystems. There is a growing number of examples for more or less successful use of these principles in earth system science, but a common systematic approach to the formulation of the relevant system boundaries, state variables and exchange fluxes has not yet emerged. Here we present a blueprint for the thermodynamically consistent formulation of box models and rigorous testing of optimality principles, in particular the maximum entropy production (MEP) and the maximum power (MP) principle. We investigate under what conditions these principles can be used to predict energy transfer coefficients across internal system boundaries and demonstrate that, contrary to common perception, these principles do not lead to similar predictions if energy and entropy balances are explicitly considered for the whole system and the defined sub-systems. We further highlight various pitfalls that may result in thermodynamically inconsistent models and potentially wrong conclusions about the implications of thermodynamic optimality principles.

The analysis is performed in an open source mathematical framework, using the notebook interface Jupyter, the programming language Python, Sympy and a newly developed package for Python, “Environmental Science using Symbolic Math” (ESSM, https://github.com/environmentalscience/essm). This ensures easy verifiability of the results and enables users to re-use and modify variable definitions, equations and mathematical solutions to suit their own thermodynamic problems.