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Key Points:

- Maximizing entropy production can be used to constrain conductances
- Assuming constant forcing results in climate-independent optimized conductances
- Dynamics in forcing do result in climate-dependent optimal conductances

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Importance of temporal variability for hydrological predictions based on the maximum entropy production principle

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Abstract This work builds on earlier work by Kleidon and Schymanski (2008) who explored the use of the maximum entropy production (MEP) principle for modeling hydrological systems. They illustrated that MEP can be used to determine the partitioning of soil water into runoff and evaporation—which determines hydroclimatic conditions around the Globe—by optimizing effective soil and canopy conductances in a way to maximize entropy production by these fluxes. In the present study, we show analytically that under their assumption of constant rainfall, the proposed principle always yields an optimum where the two conductances are equal, irrespective of rainfall rate, evaporative demand, or gravitational potential. Subsequently, we show that under periodic forcing or periodic variations in one resistance (e.g., vegetation seasonality), the optimal conductance does depend on climatic drivers such as the length of dry spells or the time of closure of stomata.

1. Introduction

1.1. Extremum Principles to Reduce the Need for Calibration

Commonly, hydrological models are calibrated with limited observations in space and time. Overparameterized models and the lack of abundant data often result in equifinality [*Beven and Freer*, 2001], i.e., a situation where different parameter sets can lead to a similar model performance. The use of optimality principles, in contrast, greatly reduces the need for calibration, as it provides an independent criteria for parameter selection, other than model performance [*McDonnell et al.*, 2007; *Schaefli et al.*, 2011; *Thompson et al.*, 2011]. Optimality based models are based on the hypothesis that, given past environmental conditions, the system of interest (e.g., catchment, river, vegetation type, or single trees) optimizes its behavior according to a candidate principle. Different objective functions have been proposed in the literature to reflect assumed organizing principles, such as minimum water stress [*Porporato et al.*, 2001; *Caylor et al.*, 2009], maximum transpiration or minimum oxygen stress [*Brolsma and Bierkens*, 2007], or maximum net carbon profit [*Schymanski et al.*, 2009].

Another principle is that of maximum entropy production (MEP) [*Paltridge*, 1979], which may be a more general principle than the ones mentioned above [*Dewar*, 2010; *Paik and Kumar*, 2010]. This thermodynamic principle can be applied to open systems that exchange mass and energy with their surroundings such as a catchment exchanging water and heat with the atmosphere and the channel network.

In atmospheric science, it has been successfully applied to estimate the atmospheric heat flux from the equator to the poles [*Paltridge*, 1979; *Lorenz et al.*, 2001]. Within hydrology, the principle has only been applied in the recent past, with varying degrees of success [*Kleidon*, 2009, 2010a, 2010b; *Porada et al.*, 2011; *Zehe et al.*, 2010; *Kleidon et al.*, 2013; *Westhoff and Zehe*, 2013; *Zehe et al.*, 2013].

Remarkably, an often reoccurring assumption is that of stationarity in forcing [e.g., *Kleidon and Schymanski*, 2008; *Dewar*, 2010; *Kleidon and Renner*, 2013], with the reasoning that "the assumption of the steady state is a simplification that may only be valid when a system is considered over sufficiently long periods" [*Kleidon et al.*, 2013]. Although it is correct that stationarity is needed for this principle (in fact, MEP determines stationarity), in the Earth system this means a statistical stationary cycle meaning that mean and variance are constant. The aim of this paper is therefore to investigate the impact of nonzero variance on MEP-derived results by exploring temporal (periodic) dynamics in forcing and system properties.

We will first give a short introduction to using the MEP principle in hydrology, then we will demonstrate analytically that the MEP solution at constant forcing is independent of the forcing itself, before investigating the effect of temporal variations in the forcing and/or system properties on predictions based on MEP.

1.2. Short Introduction to MEP

The second law of thermodynamics states that any flow or process increases the entropy S (M L^2 T^{-2} Θ^{-1}) (with Θ being temperature) of the universe. The second law also states that the entropy of any isolated system increases while it tends toward a state of maximum entropy, where all gradients have been depleted and entropy production is zero. Open systems, however, exchange entropy with their surroundings, and they can achieve a steady state where the internally produced entropy σ (M L^2 T^{-3} Θ^{-1}) equals their net entropy exchange. The MEP hypothesis states that in the presence of sufficient degrees of freedom, open systems will self-organize to maximize their entropy production σ.

Entropy production (σ) can be represented as the product of a thermodynamic force and flux and for a mass flux in the absence of temperature or pressure gradients (e.g., unsaturated flow), the relevant thermodynamic driving force can be expressed as a difference in chemical potential divided by the absolute temperature [*Kleidon*, 2010a], where chemical potential represents the sum of all relevant potentials, such as matric potential, gravitational potential, and osmotic potential:

$$\sigma = \rho Q \frac{\mu_{\mathrm{high}} - \mu_{\mathrm{low}}}{T} \tag{1}$$

where ρ is the density of water (M L^{-3}), Q is discharge (L^3 T^{-1}), μ is the chemical potential (L^2 T^{-2}), and T is the absolute temperature (Θ).

Under isothermal conditions—which we assume in this study—MEP is equivalent to maximizing power and hence we will use the terms maximum entropy production and maximum power interchangeably. Power can be described as a flux times its driving gradient, with a flux being the driving gradient divided by a resistance. A maximum in power can, in the presence of a competing flux, come about from a trade-off between maximizing a flux and maximizing its driving gradient, where the resistance is assumed to be the degree of freedom of the system.

1.3. Objective and Hypothesis

This paper builds on previous work by *Kleidon and Schymanski* [2008]. They schematized the hydrological cycle as an electrical circuit analog, where specific fluxes of water were calculated as potential differences between subsystems multiplied by respective transfer coefficients. Different chemical potentials were defined for soil water (μ_s), ocean water (μ_r), and vegetation water (μ_e), depending on the concentration of water in the respective compartment (e.g., soil moisture and relative humidity) and its gravitational potential. Assuming a constant effective rainfall rate (R (L T^{-1})) and a known runoff transfer coefficient (K_r (T L^{-1})), they demonstrated that effective soil-vegetation transfer coefficient (K_e (T L^{-1})) can be optimized in order to yield a maximum in entropy production. This was determined by first deriving the steady state chemical potential of soil water and subsequently the entropy production per unit area by evaporation σ_e [*Kleidon and Schymanski*, 2008, equations (8) and (9)]. These are given by the following:

$$\mu_s = \frac{R + K_e\mu_e + K_r\mu_r}{K_r + K_e} \tag{2}$$

$$\sigma_e = \rho K_e \left(\mu_s - \mu_e\right)^2 / T \tag{3}$$

A maximum in entropy production is obtained when $\partial\sigma_e/\partial K_e = 0$. An analytical solution (not presented by *Kleidon and Schymanski* [2008]) can be obtained by inserting equation (2) into equation (3) and taking the differential with respect to K_e:

$$\frac{\partial\sigma_e}{\partial K_e} = \frac{\rho}{T}\frac{\left(R + K_r\left(\mu_r - \mu_e\right)\right)^2\left(K_e - K_r\right)}{\left(K_r + K_e\right)^3} \tag{4}$$

Now it can be easily seen that $\partial\sigma_e/\partial K_e = 0$ has only one nontrivial solution for K_e yielding $K_e = K_r$. Thus, the optimum K_e-value is insensitive to the gradients driving the fluxes and insensitive to the total amount of water input. Or in other words, it is insensitive to climatic drivers.

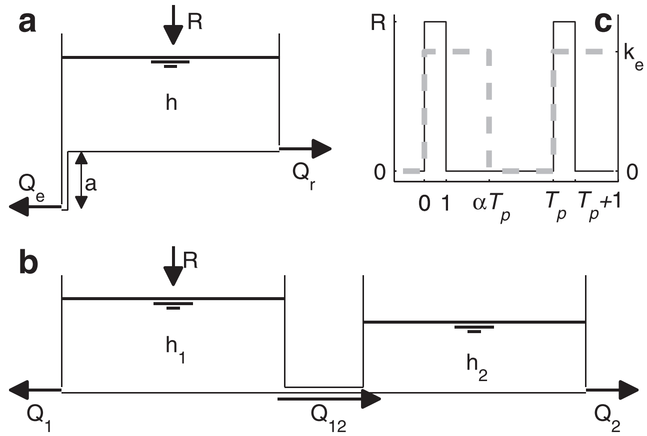

Figure 1. Model setup for (a) Cases 1 and 2 and (b) Case 3 and (c) scheme of forcing data R for Cases 1 and 3 and variation in conductance k_e for Case 2. Q refers to a water flux, R is rainfall, T is time, while h and a refer to hydraulic head.

However, in the study by *Porada et al.* [2011], the optimized transfer coefficients for the soil-vegetation flux and for runoff were different by orders of magnitude, despite using MEP. This seems indeed closer to reality, since we know that in nature, these transfer coefficients are not equal. Thus, the illustrated existence of an optimum under constant forcing [*Kleidon and Schymanski*, 2008] is not very relevant for hydrological systems; as in reality, the forcing (e.g., rainfall) varies much faster than the optimized transfer coefficients.

The aim of this paper is therefore to explore why and when the MEP principle can lead to different optimum transfer coefficients, which is inconsistent with the example given by *Kleidon and Schymanski* [2008]. We hypothesized that these differences can be explained by temporal variation in rainfall or evaporative conductance.

2. Model Setups

We explored two different model setups, of which the first one was tested under periodic forcing (Case 1) and periodic oscillations in evaporative conductance (Case 2), while the second model was only tested under periodic forcing (Case 3). For each case we considered only one degree of freedom (the conductance of one flux), which we optimized by maximizing the entropy production by its corresponding flux (expressed as power per unit area). The other conductances were given a fixed value.

2.1. Case 1

In Case 1, we used the same model as *Kleidon and Schymanski* [2008], which we translated into a single bucket model (Figure 1a). In our setup all chemical potentials are determined as a water head ($h = \mu/g$ (L)) and the transfer coefficient as a conductance ($k = gK$ (T^{-1})), with g being the gravitational acceleration (L T^{-2}). Compared to the notation in equations (2)–(4), we used $\mu_s = gh$, $\mu_r = 0$, and $\mu_e = -ga$, with h being the water level in the reservoir (L) and a being the additional potential driving evaporation (L). The mass balance per unit area for this model is given by the following:

$$\frac{\mathrm{d}h}{\mathrm{d}t} = R - Q_r - Q_e \tag{5}$$

where R, Q_r, and Q_e are the effective rainfall, specific runoff, and evaporation (L T^{-1}), with $Q_r = hk_r$ and $Q_e = (h + a)k_e$, where k_r and k_e are the conductance for runoff and evaporation (T^{-1}).

In Case 1, we used a fixed value for k_e and a, and periodic rainfall (R) while optimizing k_r to maximize power P_r (M T^{-3}). R was implemented as a fixed input that was added as a pulse of length 1T after each period T_p (Figure 1c). P_r was defined as the average power per unit area produced by Q_r over period T_p and is given by the following:

$$P_r = \frac{1}{T_p}\int_0^{T_p} \rho Q_r(t) g h(t)\mathrm{d}t = \frac{\rho g k_r}{T_p}\int_0^{T_p} h(t)^2\mathrm{d}t \tag{6}$$

We hypothesized that the periodic forcing tested in Case 1 was the main reason for the differences in conductances obtained by *Porada et al.* [2011].

2.2. Case 2

For Case 2, we used the same model setup as for Case 1, but now with constant R and varying k_e. While k_r represents hydraulic conductivity which was assumed constant during each model run, k_e represents the effective conductance of the soil-plant-atmosphere pathway, which varies diurnally due to stomatal regulation or seasonally due to variations in leaf area index.

During the simulations, R, k_r, and a were kept constant while k_e was set to a predefined value for $t = 0$ to αT_p and to zero for $t = \alpha T_p$ to T_p with α being the temporal fraction of stomata opening (Figure 1c). The parameter k_e was optimized for different values of α by maximizing the time integral of power related to evaporation:

$$P_e = \frac{\rho g k_e}{T_p} \int_0^{\alpha T_p} (h(t) + a)^2 \, \mathrm{d}t \tag{7}$$

2.3. Case 3

In Case 3, we explore the effect of periodic input for a model similar to the one by, e.g., *Lorenz et al.* [2001] or *Kleidon* [2010a] describing effective atmospheric heat transport from the equator to the poles. Within hydrology, such a model can be interpreted as a double domain model. Double domain models are often used to connect the macropore and matrix domains in the unsaturated zone. However, it is usually difficult to obtain estimates of parameters that adequately describe the interaction between the two domains. In this setup we coupled two reservoirs, of which one receives precipitation, while both lose water (representing drainage and evaporation; Figure 1b). The mass balances of both reservoirs are given by the following:

$$\frac{\mathrm{d}h_1}{\mathrm{d}t} = R - Q_1 - Q_{12} \quad \text{and} \quad \frac{\mathrm{d}h_2}{\mathrm{d}t} = Q_{12} - Q_2 \tag{8}$$

where h_1 and h_2 are the water levels in reservoirs 1 and 2, respectively. Q_1 and Q_2 are the specific fluxes out of the reservoirs 1 and 2 and Q_{12} is the specific flux between the two reservoirs. They are given by $Q_1 = h_1 k_1$, $Q_2 = h_2 k_2$, and $Q_{12} = \left(h_1 - h_2\right) k_{12}$, respectively. k_1 and k_2 were assumed to be known constants, while k_{12} was optimized to maximize power due to Q_{12}, given by

$$P_{12} = \frac{\rho g k_{12}}{T_p} \int_0^{T_p} \left(h_1(t) - h_2(t)\right)^2 \, \mathrm{d}t \tag{9}$$

The same input scenarios for R as in Case 1 were used.

3. Results and Discussion

3.1. Case 1

Using the same model as *Kleidon and Schymanski* [2008], but now optimizing k_r subject to periodic forcing R led, as hypothesized, to different optimal conductances (Figure 2). For Case 1, a constant input resulted indeed in maximum power at $k_r = k_e = 10^{-3}\ \mathrm{T}^{-1}$, but when dry spells were introduced ($T_p > 1\mathrm{T}$), a second optimum appeared at much larger values of k_r. For large periodicities this second optimum eventually becomes the global optimum (Figure 2b).

This second optimum develops when in-between two pulses the reservoir becomes empty. When this happens, it is more favorable in this thermodynamic approach to empty the reservoir fast by increasing the conductance. In this way most of the water is used to produce power by runoff and less by the competing evaporative flux. The effect was so strong that the optimal solution for return periods of $R \geq 50$ T gave an empty reservoir for more than 90% of the time, which is in accordance with runoff production in arid areas. The reason that the optimum k_r is not infinitely large, is that there is still a trade-off between the flux and the gradient driving the flux.

The climate dependence of this model is not only reflected in the length of the dry spell, but also in the ratio of a to R. This ratio is the same for Figures 2b and 2c ($a/R = 5$ T), resulting in exactly the same optimal k_r value of 0.17 T^{-1}. The optimum k_r value was larger for larger ratios (Figure 2a; $a/R = 10$ T, $k_r = 0.23\ \mathrm{T}^{-1}$) and smaller for smaller ratios (Figure 2d; $a/R = 2.5$ T, $k_r = 0.13\ \mathrm{T}^{-1}$). These unique k_r values for each a/R-ratio results also in a unique evaporation index (Q_e/R), which may be a first step toward reconciling the Budyko curve.

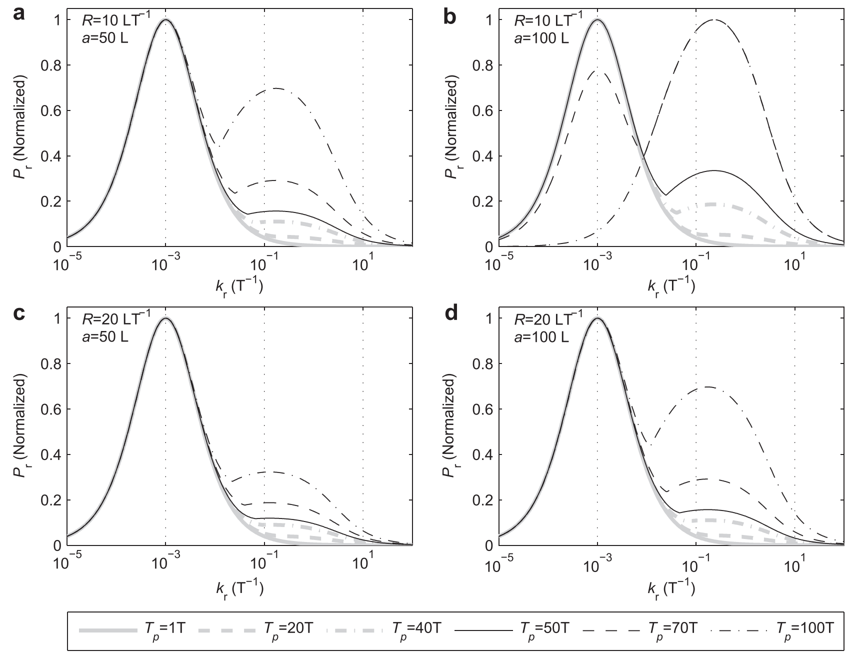

Figure 2. (a–d) Runoff conductance k_r versus normalized power P_r produced by runoff for Case 1 with evaporative conductance $k_e = 10^{-3}$ T^{-1}. a is the additional head driving evaporation and R is rainfall with a duration of 1T for each period T_p. Each line is normalized by its own maximum.

3.2. Case 2

For Case 2, we tested the effect of periodic variations in k_e, representing seasonal vegetation dynamics or diurnal opening and closing of stomata. The evaporative flux was periodically turned on and off for different fractions of the period T_p, while the forcing was kept constant over time. The optimum k_e value was determined for a given fraction of opening (α). Without closing ($\alpha = 1$) maximum power is produced for $k_e = k_r = 10^{-3}$ T^{-1}, while for any values of $\alpha < 1$, $k_e > k_r$ (Figure 3). The optimal k_e values do also depend on the total period T_p, with smaller k_e values for longer periods (compare gray and black lines in Figure 3). Considering that α and T_p vary with climate (e.g., sunlight, relative humidity, temperature, and soil moisture), the optimal value of k_e would also be climate dependent.

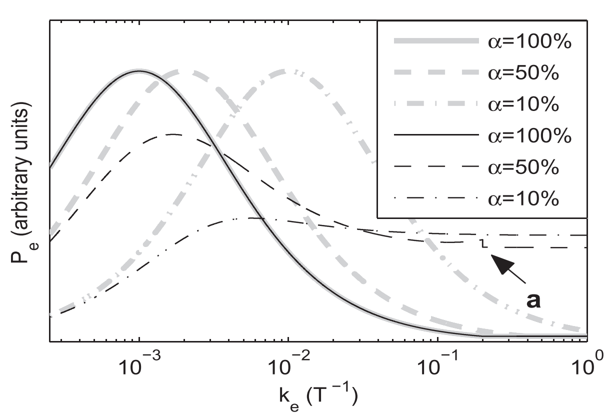

Figure 3. Evaporative conductance k_e versus power produced by evaporation (Q_e) for $k_r = 10^{-3}$ T^{-1}, $a = 50$ L, and $R = 10$ L T^{-1}. Grey lines were simulated with $T_p = 1$ T and black lines with $T_p = 5000$ T. Note that the jump at point **a** happens when $k_e a > R$ and T_p is large enough to let the reservoir fall dry; for a dry reservoir Q_e reduces to R.

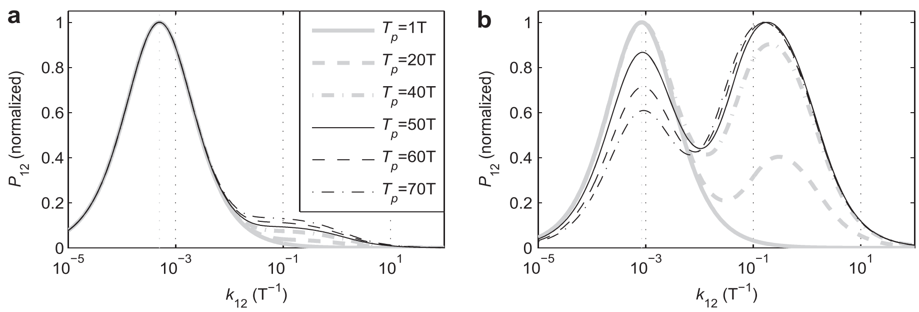

Figure 4. Conductance k_{12} versus normalized power produced by Q_{12} for Case 3 with (a) $k_1 = k_2 = 10^{-3}$ T^{-1} and (b) $k_1 = 5 \cdot 10^{-3}$ T^{-1} and $k_2 = 10^{-3}$ T^{-1}. Input R is a pulse of 10 L T^{-1} with each line being a different periodicity T_p.

3.3. Case 3

Assuming constant forcing, the optimum k_{12} can, for Case 3, also be obtained analytically, similarly to Case 1. The equilibrium water levels are given by the following:

$$h_1 = \frac{R\left(k_{12} + k_2\right)}{k_1k_2 + k_1k_{12} + k_2k_{12}},\ h_2 = \frac{Rk_{12}}{k_1k_2 + k_1k_{12} + k_2k_{12}} \tag{10}$$

Combining equations (9) and (10) and differentiating gives

$$\frac{\partial P_{12}}{\partial k_{12}} = \frac{\rho g(Rk_2)^2\left(k_1k_2 - k_1k_{12} - k_2k_{12}\right)}{(k_1k_2 + k_1k_{12} + k_2k_{12})^3} \tag{11}$$

Equation (11) is zero for the nontrivial solution $k_{12} = k_1k_2/\left(k_1 + k_2\right)$. Thus, assuming constant input, this solution is also independent of the total amount of rainfall.

Under periodic forcing, the sensitivity depends on the given values for k_1 and k_2 (Figure 4). Using the same values for k_1 and k_2, a periodic input did not result in a shift in optimum k_{12} (Figure 4a). However, when $k_1 > k_2$ a second optimum developed with increasing dry periods. The reason for this behavior is in principle the same as in Case 1: The gradient that drives Q_{12} becomes zero in-between two pulses, implying that in this model setup, $h_1 = h_2$. This is only possible when the first reservoir drains faster than the second (which is the case when $k_1 > k_2$), since only the first reservoir received the input from rainfall. In a double domain model, one can interpret reservoir 1 as the macropore and reservoir 2 as the matrix that receives its water mainly from interaction with the macropore. Using this interpretation, k_1 is indeed larger than k_2.

4. Conclusion and Outlook

The principle of maximum power—and equivalent to that the MEP principle—is a promising hypothesis, which, if true, could be used to estimate model parameters without the need for calibration. Although a promising hypothesis, there are still many unresolved issues.

While *Kleidon and Schymanski* [2008] showed how the principle could be used to determine the partitioning between evaporation and runoff, we showed that under their assumption of constant forcing the optimal conductances are independent of the amount of rainfall and independent of the extent of the driving gradients. We furthermore showed that adding periodicity in forcing or conductances does result in climate-dependent optimal conductances. We consider this as an important finding, since such dynamics have been ignored in several studies [e.g., *Lorenz et al.*, 2001; *Dewar*, 2010; *Kleidon et al.*, 2013; *Kleidon and Renner*, 2013].

Our results are a proof of concept. However, to test the principle against data, more realistic potential gradients are needed, as opposed to the well-mixed reservoirs and idealized gradients in our model. A starting point could be to infer matrix potentials from soil water retention parameterizations [see, e.g., *Porada et al.*, 2011]. Model structure 2 can be a representative for a double domain model. However, it remains to be seen, whether such MEP predictions of effective conductivities of matrix versus macropore domains can reproduce observations [*Westhoff and Zehe*, 2013].

We would like to stress that this paper by no means represents a confirmation or otherwise of the MEP hypothesis. The results presented here merely suggest that model results based on this hypothesis are likely sensitive to periodicity in forcing and possible dynamics of the optimized degrees of freedom (e.g., k_e). Before rigorous testing of the MEP hypothesis can be done, a few open issues have to be resolved, such as determination of the relevant driving gradients, degrees of freedom, and constraints of a given system. However, we believe firmly that the potential benefits (e.g., reduction of the need for calibration) justify the efforts required to take this approach a step further.

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