Interactive comment on “Optimality and inference in hydrology from entropy production considerations: synthetic hillslope numerical experiments” by S. J. Kollet

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1 Summary

The stated objective of the paper is to test the hypothesis that “if a single atmospheric time series is repeatedly applied over a hillslope until dynamic equilibrium is reached, then the hillslope will tend toward an optimized state of exchange, when entropy or power production is maximized”. This is attempted by running a spatially resolved (2D) hydrological hillslope model and computing associated thermodynamic variables such as water potential gradients and isothermal entropy production, represented as power related to fluxes of water down a water potential gradient, i.e. flux multiplied by the gradient. The model was run for a synthetic hillslope using the same atmospheric forcing and soil properties, but varying the saturated hydraulic conductivity ($K_{\text{sat}}$) by five orders of magnitude. Two sets of simulations were performed, one with spatially homogeneous $K_{\text{sat}}$ and one where $K_{\text{sat}}$ was randomly perturbed around the prescribed mean value. The simulations resulted in the occurrence of a water table at low values of $K_{\text{sat}}$, whereas a water table was absent for higher values. The author found that the presence of a water table had a strong influence on the pattern of water flow power in the simulation domain, with average power expressing two maxima with increasing
$K_{\text{sat}}$, one in the presence and one in the absence of a water table. The author also found clear vertical and horizontal zonations of low and high net power across the hill-slope cross-sections and very strong small-scale heterogeneity between grid cells. In a second step, the author attempted to deduce effective hillslope-scale conductances and potential gradients from the detailed small scale simulations. This was done by using the equation for flow as a function of conductance and head gradient and the equation for power as a function of flow and head gradient. Using the simulated net flow rates and net power, the author obtained two equations with two unknowns, an effective head gradient and an effective conductance. When plotting net power as a function of effective conductance, the author obtained a single maximum, as opposed to two maxima when plotting as a function of saturated hydraulic conductivity. This was interpreted as evidence for maximisation of power at the hillslope scale and for the utility of the MEP principle as inference tool.

2 General comments

The paper contains a range of interesting results and discussion, but I believe that the insights with respect to maximum entropy production or power presented in this study could be enhanced a lot and need some clarifications. I also found some potential flaws that need to be dealt with.

First of all, the author did not explain how water fluxes are calculated in the model, whether hydraulic heads used for calculation of entropy production include gravitational potential and how fluxes out of the domain were modelled. Power (representative of entropy production) is only calculated for internal flow processes, no calculation of entropy exchange between grid cells or for water exchange across the boundaries is presented. As the author points out on P. 5126 L1, entropy production or power is a positive quantity by definition, so I am uncertain how to interpret Fig. 2 with positive and...
negative values of average net power. In fact, the big red block with sharp boundaries in Fig. 2a looks like an artefact to me and should be analysed/discussed in more detail. At steady state, entropy in each grid cell must be constant, meaning that the entropy produced internally must equal the net export of entropy to the surroundings Schymanski et al. (2010). For a dynamic steady state, as assumed in the present paper, this must be true for long-term average entropy balance, so I believe that a detailed calculation of the entropy balance, not only entropy production, may give an additional indication of the consistency in the calculations.

Secondly, the author presents the mere existence of a maximum in power with varying conductance as indication that “power is indeed maximized” in the simulations. For this statement to be substantiated, it would be necessary to demonstrate that the conductivity resulting in maximum power is indeed the one a hillslope naturally assumes. This has not been done and hence all that could be concluded from this study is that maxima exist along the range of simulated conductivities. In this context, I am uncertain how to interpret the deduced “effective” conductivity and the fact that only one maximum in power is expressed over the range of calculated effective conductivities. According to P. 5137 L4, the author calculates the effective conductivity as the ratio of average power to the square of average hydraulic head difference. This derivation seems flawed, as the mean of a ratio is not equal to the ratio of two means, and the mean of a square is not equal to the square of a mean. For a correct calculation, the variances and covariances of the variables need to be considered.

I also failed to see the merit of deducing effective conductances and pressure heads from the numerical simulations, given that both of these vary in space and time. I think that derivation of effective static soil properties and effective hillslope or catchment geometry would be more useful. Or, even better, if a global optimum in $K_{sat}$ with respect to macroscopic power or entropy production exists, it would be very interesting to assess if real hillslopes tend towards such an optimal value.

I hope that these and the below step-by-step comments will help to improve the
manuscript and make it an inspiring and useful addition to the scientific literature.

3 Specific comments

1. Throughout: The use of the term optimization is confusing. Entropy production is maximized by optimization of some system properties such as effective conductance or spatial arrangement. If entropy production were to be optimized, as stated in this manuscript, I would expect that something else was the objective function to be maximized or minimized, while entropy production was the adjustable lever. On P5125L3 the term “entropy production optimization (EPO)” is introduced. How does this differ from “maximum entropy production (MEP)”?

2. Throughout: It would be helpful to remind the reader every now and then what the different abbreviations mean, e.g. S1 and S2 being homogeneous or heterogeneous $K_{\text{sat}}$ respectively.

3. Throughout: Please do not use the word “chaos” when referring to heterogeneity. Chaos has a specific mathematical definition and could confuse readers.

4. P5124L13: inference tool

5. P5125L10: The property of being well mixed or not is unrelated to being stationary or non-linear. To avoid confusion, this section should be re-written and a discussion of macroscopic variables could also be added here.

6. P5125L15–: The discussion of entropy production and associated variables is very confusing. What kind of entropy production is maximised, what are relevant system boundaries? The units given here are not consistent: Chemical potential should be energy per mass or per mole, entropy production should be energy per Kelvin per time, power should be energy per time by definition. Using the notation
here, energy should be ML$^2$T$^{-2}$, but this is neither reflected in the units of entropy production, nor in the chemical potential or power.

7. P5126L5: Clearer formulation: $\lambda$ is optimised to maximise $P$.

8. P5126L14–16: Kleidon and Schymanski (2008) did not show that entropy is maximised, they hypothesised that this might be the case. I was hoping that the present manuscript would test this hypothesis.

9. P5126L24: Linearity is not needed to use an idealized box model.

10. P5127L6–10: Need to explain what are the state variables that are supposed to be optimised for maximum entropy production or power.

11. P5127L16: 2D horizontally or vertically?

12. P5128L10–16: A conceptual drawing of the system boundaries and exchange would be helpful here. Why no-flow conditions? Where does the water go? How are the fluxes within the system and across boundaries computed?

13. P5128L17: maximum in P (not optimum)

14. P5131L16: This implies no drainage, however on P5529L7 it was mentioned that drainage does occur in some simulations.

15. P5131L19: What does it mean that infiltration equals negative evaporation? Why negative?

16. P5133L7–11: Would this stepwise representation of topography lead to an over-estimation of power compared to a more smooth representation?

17. P5133L15–19: I was not able to follow here. I did not see the circulation patterns or understand whether these bands in Fig. 2 have a meaning or are an artefact.
18. P5134L8–9: I see no evidence for the statement that there is some sort of maximization in the critical zone. Figs. 4 and 6 show that there are maxima as $K_{sat}$ is varied, but the evidence that the hillslope tends towards such states is not given.

19. P5135L13: These circulation cells sound interesting, but I was not able to see them.

20. P5135L15: This is interesting. Does a random perturbation generally result in larger effective conductance, then?

21. P5136L1–3: This has actually been done in Schymanski et al. (2010): A “microscopic” spatially resolved ecohydrological model was transferred into a macroscopic 2-box model with effective parameters, which were optimised using the MEP principle, and the model results turned out to be very similar to the microscopic model simulations. Could this be attempted here as well?

22. P5136L22: The equation given here is wrong, as the mean of a quotient is not equal to the quotient of two means. The mean $\Delta H$ is equal to the mean of $P/q$, not to the mean of $P$ divided by the mean of $q$, as long as $P$ and $q$ are not independent variables. Therefore, the interpretation of these results is likely flawed.

23. P5137L4: Again, mean $\lambda$ should be calculated as the mean of all values of $\lambda$, not as the mean of $P$ divided by the square of the mean $H$.

24. P5137L18–20: This conclusion seems unjustified. All the figure shows is that there is a maximum but not that the hillslope tends towards such a maximum.

25. P5138L9–10: Again, the results do not indicate to me that a hillslope tends towards an MEP state, they just show that there are maxima in power for certain values of saturated hydraulic conductivity.
26. P5138L20–24: I don’t see the use of deriving “effective gradients in case of known net fluxes”. Both fluxes and gradients vary in time, so what would we gain by this?

27. P5140L9–11: It would be interesting to add an entropy balance to these calculations, in order to test whether the theoretical framework is indeed consistent.

28. Fig. 1: Why qualitative and not e.g. a logarithmic colour scheme? Surely, the colour scheme does follow some mathematical transformation anyway. What is the meaning of evaporation greater 0 and infiltration lower than 0 for discharge vs. recharge? This distinction did not make any sense to me.

29. Fig. 2: I had to look twice in the original manuscript to verify that the red bar was not a printout error. It may be good to mention in the caption that this is the actual result, and discuss in the text what caused it. Here, the scale could also be made quantitative.

30. Fig. 6: The arrangement of a-d is different to Fig. 4, while the shape of Fig. 6a is similar to Fig. 4a. Is this coincidence or a mix-up of the axes labels?

References
