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Linking landscape structure and rainfall runoff behaviour in a thermodynamic optimality context

Erwin Zehe (1), Uwe Ehret (1), Theresa Blume (2), Axel Kleidon (3), Ulrike Scherer (1), and Martijn Westhoff (4)

(1) Institute of Water Resources and River Basin Management, Karlsruhe Institute of Technology KIT, Karlsruhe, Germany (erwin.zehe@kit.edu), (2) GFZ German Research Centre for Geosciences, Section 5.4 Hydrology, Potsdam Germany, (3) Max-Planck-Institut für Biogeochemie, Jena, Germany, (4) Hydraulics in environmental and civil engineering, University of Liege, Belgium

The fact that persistent spatial organization in catchments exists has inspired many scientists to speculate whether this is the manifestation of an underlying organizing principle. In line with these studies we developed and tested a thermodynamic framework to link rainfall runoff generation and self-organization in catchments. From a thermodynamic perspective any water mass flux is equal to a "potential gradient" divided by a "resistance", and fluxes deplete due to the second law of thermodynamics their driving gradients. Relevant potentials controlling rainfall runoff are soil water potentials, piezometric heads and surface water levels and their gradients are associated with spatial differences in associated forms of free energy. Rainfall runoff processes thus are associated with conversions of capillary binding energy, potential energy and kinetic energy. These conversions reflect energy conservation and irreversibility as they imply small amounts of dissipation of free energy into heat and thus production of entropy. Energy conversions during rainfall runoff transformation are, though being small, nevertheless of key importance, because they are related to the partitioning of incoming rainfall mass into runoff components and storage dynamics. This splitting and the subsequent subsurface dynamics is strongly controlled by preferential flow paths, which in turn largely influence hydrologically relevant resistance fields in larger control volumes. The field of subsurface flow resistances depends for instance on soil hydraulic conductivity, its spatial covariance and soil moisture. Apparent preferential pathways reduce, depending on their density, topology and spatial extent, subsurface flow resistances along their main extent, resulting in accelerated fluxes against the driving gradient. This implies an enlarged power in the subsurface flux thereby either an enlarged free energy export from the control volume or an increased depletion of internal driving gradients, and thus a faster relaxation back towards local thermodynamic equilibrium. Thermodynamic optimality principles allow for a priory optimization of the resistance field at a given gradient, not in the sense how they exactly look like but in the sense how they function with respect to export and dissipation of free energy associated with rainfall runoff processes. Based on this framework we explored the possibility of independent predictions of rainfall runoff, in the sense that the a-priory optimum model structures should match independent observations. We found that spatially organized patterns of soils and macropores observed in two distinctly different landscapes are in close accordance with thermodynamic optima expressed either by minimized relaxation times towards local thermodynamic equilibrium in cohesive soils or as steady state in the potential energy of soil water in non-cohesive soils. Predicted rainfall runoff based on the two optimized model structures was in both catchments in acceptable accordance with independent discharge observations.

However, the nature of these optima suggests there might be two distinctly different thermodynamically optimal regimes of rainfall runoff behaviour. In the capillary- or c–regime, free energy dynamics of soil water is dominated by changes in its capillary binding energy, which is the case for cohesive soils. Soil wetting during rainfall in the c-regime implies pushing the system back towards LTE, especially after long dry spells. Dead ended macropores (roots, worm burrows which end in the soil matrix) act as dissipative wetting structures by enlarging water flows against steep gradients in soil water potential after long dry spells. This implies accelerated depletion of these gradients and faster relaxation back towards LTE during rainfall runoff. In the c-regime several optimum macropore densities with respect to maximization of net reduction of free energy exist. This is because the governing equation is a second order polynomial of the wetting rate, which depends on macropore density, the slope of the soil water retention curve, topography and depth to groundwater. An uncalibrated long term simulation of the water balance of the 3.5 km^2 Weiherbach catchment based on the first optimum macroporosity performed almost as well as the best fit when macroporosity was calibrated to match rainfall runoff.

In the other regime called potential- or p-regime, free energy dynamics of soil water is dominated by changes in

its potential energy, which applies to non-cohesive soils and a pronounced topography. Soil wetting during rainfall in the p-regime implies to push the system away from LTE. This can be compensated by preferential pathways which connect directly to the riparian zone or the groundwater body, because these drainage structures enhance export of potential energy from the critical zone. However, in the p-regime no local optimum exists because potential energy reduction rates scale linearly with the drainage rate (there is at best an optimum at the margin of the parameter space). Nevertheless, in this case one can define a "distinguished" density of vertical and lateral preferential flow paths that assures steady state conditions of the potential energy balance of the soil. This applies when average storage of potential energy is compensated by average potential export . When applying this idea to the Mallalcahuello catchment in Chile model, which is characterized by non-cohesive soils, high annual rainfall and steep terrain, simulations performed close to the value that yielded the best fit of rainfall runoff behaviour obtained during a calibration exercise. Secondly this idea allowed a robust a priory estimate of the annual runoff coefficient in accordance with long term observations.