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HESS Opinions: From response units to functional units: a thermodynamic reinterpretation of the HRU concept to link spatial organization and functioning of intermediate scale catchments

E. Zehe[1], **U. Ehret**[1], **L. Pfister**[2], **T. Blume**[3], **B. Schröder**[4,5], **M. Westhoff**[1], **C. Jackisch**[1], **S. J. Schymanski**[6], **M. Weiler**[7], **K. Schulz**[8], **N. Allroggen**[9], **J. Tronicke**[9], **L. van Schaik**[4], **P. Dietrich**[10], **U. Scherer**[1], **J. Eccard**[5,9], **V. Wulfmeyer**[11], and **A. Kleidon**[12]

[1]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany
[2]Centre de Recherche Public – Gabriel Lippmann, Belvaux, Luxembourg
[3]GFZ German Research Centre for Geosciences, Potsdam, Germany
[4]Technische Universität Braunschweig, Braunschweig, Germany
[5]Berlin-Brandenburg Institute of Advanced Biodiversity Research (BBIB), Berlin, Germany
[6]Swiss Federal Institute of Technology, Zurich, Switzerland
[7]University of Freiburg, Freiburg, Germany
[8]University of Natural Resources and Life Sciences, Vienna, Austria
[9]University of Potsdam, Potsdam, Germany
[10]Helmholtz Centre of Environmental Research, Leipzig, Germany
[11]Universität Hohenheim, Hohenheim, Germany
[12]Max Planck Institute for Biogeochemistry, Jena, Germany

Correspondence to: E. Zehe (erwin.zehe@kit.edu)

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Abstract. According to Dooge (1986) intermediate-scale catchments are systems of organized complexity, being too organized and yet too small to be characterized on a statistical/conceptual basis, but too large and too heterogeneous to be characterized in a deterministic manner. A key requirement for building structurally adequate models precisely for this intermediate scale is a better understanding of how different forms of spatial organization affect storage and release of water and energy. Here, we propose that a combination of the concept of hydrological response units (HRUs) and thermodynamics offers several helpful and partly novel perspectives for gaining this improved understanding. Our key idea is to define functional similarity based on similarity of the terrestrial controls of gradients and resistance terms controlling the land surface energy balance, rainfall runoff transformation, and groundwater storage and release. This might imply that functional similarity with respect to these specific forms of water release emerges at different scales, namely the small field scale, the hillslope, and the catchment scale. We thus propose three different types of "functional units" – specialized HRUs, so to speak – which behave similarly with respect to one specific form of water release and with a characteristic extent equal to one of those three scale levels. We furthermore discuss an experimental strategy based on exemplary learning and replicate experiments to identify and delineate these functional units, and as a promising strategy for characterizing the interplay and organization of water and energy fluxes across scales. We believe the thermodynamic perspective to be well suited to unmask equifinality as inherent in the equations governing water, momentum, and energy fluxes: this is because several combinations of gradients and resistance terms yield the same mass or energy flux and the terrestrial controls of gradients and resistance terms are largely independent. We propose that structurally adequate models at this scale should consequently disentangle driving gradients and resistance terms, because this optionally allows equifinality to be partly reduced by including available observations, e.g., on driving gradients. Most importantly, the thermodynamic perspective yields an energy-centered perspective on rainfall-runoff transformation and evapotranspiration, including fundamental limits for energy fluxes associated with these processes. This might additionally reduce equifinality and opens up opportunities for testing thermodynamic optimality principles within independent predictions of rainfall-runoff or land surface energy exchange. This is pivotal to finding out whether or not spatial organization in catchments is in accordance with a fundamental organizing principle.

1 Introduction

Almost 30 years ago Dooge (1986) identified the organized complexity of intermediate-scale catchments between 5 and 250 km^2 as a cardinal problem in hydrological research. Dooge (1986) defined them as systems that exhibit a considerable degree of both spatial organization and stochastic heterogeneity, being too large for a fully deterministic treatment yet too small for a simplified conceptual treatment. Despite the great progress that has been achieved in hydrology of hillslopes and at the scale of organized simplicity (Dooge, 1986), we feel that our understanding at the intermediate scale of organized complexity is still rather incomplete. Why so? These systems are already too large and too heterogeneous to take real advantage from applying physically based models, as already pointed out by Beven (1989). This is due to the absence of the required detailed data (e.g., on patterns of soil hydraulic functions, the topology of preferential flow paths, the physiology of apparent vegetation), because their exhaustive characterization at intermediate scales is severely limited by present measurement technology and experimental design (Beven, 2006; Kirchner, 2006, Zehe et al., 2007). We of course acknowledge that parameter sets of "physics-based models" can be derived by calibration/inverse modeling as done for Hydro-Geo-Sphere (Perez et al., 2011), Mike She (Christiaens and Feyen, 2001, 2002) or CATFLOW (Klaus and Zehe, 2010). However, these efforts lead (unsurprisingly) to the same problems encountered in the calibration of conceptual models. On the one hand, we obtain either effective soil hydraulic functions that jointly represent matrix and preferential flow (Troch et al., 1993; Hopp and McDonnell, 2011): we are then stuck with non-commensurable parameters that cannot be constrained using measured data derived within multistep outflow experiments. On the other hand, if we decide to disentangle matrix and preferential flow, we face a strong equifinality in acceptable model structures, also because a large set of different flow network topologies produce similar response behavior (Weiler and McDonnell, 2007; Klaus and Zehe, 2010; Wienhöfer and Zehe, 2014).

Intermediate-scale catchments with a strong spatial organization are, unfortunately, also too small for averaging out errors of simplified conceptual model approaches (as they tend to do according to Dooge (1986) at the scale of organized simplicity). Both the land surface energy balance and rainfall runoff generation reflect fingerprints of how the partly organized and partly heterogeneous patterns of soils and network-like structures (surface and subsurface preferential flow paths, vegetation, or structures associated with surface atmospheric turbulence) nonlinearly interact with the prevailing meteorological states and forcing (Schulz et al., 2006). These "structure–process" interactions cause, depending on the pattern of system states, threshold or emergent behavior (Zehe and Sivapalan, 2009): due to either (a) the onset of preferential flow and potentially subsurface pipe flow, reducing overland flow formation (Buttle and McDonald, 2002; Zehe et al., 2005; Tromp-van Meerveld and Weiler, 2008; Wienhöfer et al., 2009; Fujimoto et al., 2011), (b) the rapid mobilization of pre-event water due to pressure transduction (e.g., Bonell et al., 1990; Sklash et al., 1996), or (c) the switch between either atmospheric or land surface controlled evapotranspiration (ET, McNaughton and Jarvis, 1983; Dooge, 1986; Seneviratne et al., 2010). However, we lack suitable theoretical concepts to explain these threshold changes and emergent behavior, and to represent them in conceptual models.

Today, almost 30 years after the problem of organized complexity was identified, there is still a gap at the intermediate scale with respect to (a) our understanding, (b) structurally adequate models that step beyond input–output predictions, and (c) experimental strategies to collect useful data in a representative way to support modeling and understanding (Kirchner, 2006; McDonnell et al., 2007). As a consequence, hydrological practice often avoids operational flood forecasts in intermediate-scale catchments not only because of the highly uncertain rainfall predictions but also because of the deficiencies of rainfall runoff models and data collection strategies that prevail at this scale. Here, we stipulate that a better understanding of how different forms of spatial organization affect storage and release of water and energy across scales is essential for narrowing this gap. The key to gain such an improved understanding is in our opinion a reinterpretation of the concept of hydrological response units (HRUs, Flügel, 1996) – which we greatly appreciate – from a thermodynamic perspective (Kondepudi and Prigogine, 1998). The proposed reinterpretation offers alternative perspectives:

- for defining functional similarity based on similarity of terrestrial and atmospheric controls on driving gradients and resistance terms. This implies that functional similarity is not static in the sense of a "one fits all processes" HRU, but that specific functional units (specialized HRUs) for a specific form of "water release" might exist, and operate at different scales (as explained in Sect. 2);

- for alternative experimental strategies. They rely on exemplary learning and replicate experiments and monitoring, to characterize how different forms of spatial organization control how catchments store and release water and energy (as explained in Sect. 3);
- for requirements to be met by structurally adequate models; for equifinality as an inherent part of their governing equations; for ways to partly reduce this equifinality by a systematic linkage of observations to model components representing driving gradients and resistance terms (as explained in Sects. 4.1 and 4.2);
- for assessing whether persistent spatial organization in catchments is in accordance with thermodynamic optimality principles and whether this offers opportunities for uncalibrated predictions (as explained in Sect. 4.3).

The thermodynamic perspective yields, most importantly, a consistent energy-centered perspective on rainfall runoff transformation and ET. This includes fundamental upper limits for energy fluxes associated with these processes, which might be used to reduce equifinality, and opens opportunities for testing thermodynamic optimality principles within independent predictions of rainfall runoff or land surface energy exchange.

2 Reinterpreting the HRU idea from a thermodynamic perspective

2.1 Hydrological processes from a thermodynamic perspective

Flügel (1996) defined HRUs as “distributed, heterogeneously structured entities having a common climate, land use and underlying pedo-topo-geological associations controlling their hydrological transport dynamics”. When landscapes and their spatial organization are seen as open thermodynamic systems, similar functioning identified in observations suggests a similar thermodynamic state and functionality (Reggiani et al., 1998; Rasmussen et al., 2011). A necessary step to reinterpret the HRU idea from a thermodynamic perspective is to express hydrologic fluxes in thermodynamic terms (Kleidon et al., 2013). At the very basic level, the second law of thermodynamics tells us that (potential) gradients are depleted by the fluxes that are caused by these gradients (e.g., Kleidon et al., 2013), no matter whether we deal with energy, momentum, or mass fluxes (of water, solutes or sediments). Depletion of driving gradients implies production of entropy and dissipation of free[1] energy. This direction of the second law is the foundation for expressing hydrologic fluxes (in fact any flux in physics) in the common way as a product of a conductance (or an inverse resistance, R) and a gradient[2] $\nabla\Phi$.

$$\boldsymbol{q} = -\underline{1/R}\nabla\boldsymbol{\phi} \tag{1}$$

Hydrologically relevant potentials consist of (spatio-temporal fields of) soil or air temperature, soil or plant water potentials, piezometric heads, or surface water levels driving turbulent fluxes of latent and sensible heat, fluxes of capillary soil water and soil heat, or fluxes of free water sustaining different runoff components (Table 1). The magnitude of these fluxes is determined by the set of governing equations and especially hydrologically relevant resistances, and also by thermodynamic limits such as the Carnot efficiency (Kleidon et al., 2012; Rasmussen, 2012). The resistances terms, symmetric tensors in the most general case, relate to the inverse of the soil heat conductance, or the canopy and aerodynamic resistances, or the surface roughness, or the inverse of soil hydraulic conductivity. These resistances determine dissipative energy losses along the different flow paths, and strongly reflect the degree of heterogeneity of either soil materials in the subsurface control volume or the physiology and morphology of the vegetation at the land surface. Subsurface or plant resistances furthermore depend non-linearly on soil or plant water content, which also controls soil or plant water potentials.

Isolated systems, which exchange neither mass nor energy with their environment, evolve to a “dead state” of maximum entropy due to the absence of any driving potential gradient, called thermodynamic equilibrium (TE). Open systems such as the critical zone may, however, export entropy to the environment and maintain a spatially organized configuration far from thermodynamic equilibrium (Kleidon et al., 2012).

From a thermodynamic perspective we may distinguish two different forms of water release, because they are driven by different gradients, and are thus associated with different energy conversions as well as different degrees of freedom of the system. On one hand the catchment may release water vapor to the atmosphere by means of ET. ET is tightly linked with land surface–atmosphere energy exchange, which is driven by differential radiative heating between the surface and the atmosphere, causing near surface gradients in air temperature and humidity. These gradients drive the turbulent fluxes, which are partly fed from soil water that is held by capillary forces against gravity. Vegetation acts as a “preferential flow path” for capillary water and

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[1] Which in the Oxford Dictionary is defined as a thermodynamic quantity equivalent to the capacity of a system to perform work: i.e., to accelerate a (water) mass (as overland flow), to lift a (water) mass against gravity (as capillary rise), or to enlarge a potential gradient.

[2] To be precise, fluxes are driven by potential gradients, i.e., gradients in intensive state variables such as temperature or matric potentials, which are continuous at interfaces and non-additive. Extensive state variables such as soil moisture, internal energy, or mass may on the contrary be discontinuous at interfaces and are additive.

Table 1. Gradients and resistances determining fluxes/storage of water and energy as well as their landscape controls, with special emphasis on the influence of connected network-like structures that reduce resistances.

Processes	Gradient	Landscape control	Resistance	Network-like structure
Transpiration	Vapor pressure canopy–atmosphere (due to radiative heating)	Canopy albedo and temperature Aspect and slope Air vapor pressure Soil water potential Wind speed	Canopy and boundary layer resistances, root resistance, plant physiology	Canopy structure, leaf area index (LAI), root network topology
Evaporation	Vapor pressure soil–atmosphere (due to radiative heating)	Soil albedo and temperature Aspect and slope Soil water content & soil water retention curve Wind speed	Inverse of soil hydraulic conductivity Boundary layer resistance	Pore network
Sensible heat flux	Temperature surface–atmosphere	Soil albedo and temperature Aspect and slope Surface roughness Air temperature Wind speed	Turbulent/laminar boundary layer resistance	
Soil heat flux	Soil temperature	Soil albedo and temperature Aspect and slope Heat capacity Soil water content	Inverse of soil thermal conductivity content	Advective heat flux
Surface runoff	Overland flow depth	Surface topography and permeability	Surface roughness (incl. plants and debris),	Rill network topology & spec. flow resistance
Infiltration	Soil water potential	Soil water retention curve, soil water content, depth to groundwater	Inverse of hydraulic conductivity, soil water content	Macropore network topology & spec. flow resistance
Root water uptake	Water potential soil–root	Rooting depth Fine root distribution Canopy water demand Soil water content Depth to groundwater	Root system resistance Inverse of hydraulic conductivity	Root network Macropore network
Subsurface storm flow	Gradient in free water table (gravitational potential gradient)	Bedrock topography and permeability	Inverse of hydraulic conductivity, soil water content	Lateral pipe network & spec. flow resistance
Groundwater flow	Piezometric head	Aquitart topography, specific storage coefficient	Inverse of hydraulic permeability	Fracture network topology & spec. flow resistance

groundwater into the atmosphere, as plant roots may extract soil water against steep gradients in soil water potential and thus shortcut dry topsoil layers, which block bare soil evaporation considerably. The plant's metabolism that sustains this preferential flow path is maintained by photosynthesis, which links to plant gas exchange (Schymanski et al., 2009) controlled by plant physiology (root water uptake, plant water transport, stomata conductance). Entropy production in a catchment is dominated by ET due to the large specific heat of vaporization (Kleidon, 2012), while entropy export is sustained by outgoing long wave radiation and turbulent heat fluxes (Kleidon, 2012).

Alternatively, the catchment may release liquid water as stream flow. Stream flow and its generation are driven by gravity, and feed either from direct rainfall-runoff transformation or from non-capillary water which is temporarily stored in the aquifer (or in the subsurface) and eventually released to the stream. Also the mass fluxes during rainfall runoff processes are tightly linked to free energy conversions, namely of capillary binding energy of soil water (in fact chemical energy), potential energy, and kinetic energy of soil and/or surface water. Although small when compared to the surface energy balance, these energy conversions are of key importance. This is because they are related to the partitioning of incoming rainfall mass into runoff components and storage dynamics (Zehe et al., 2013) and reflect energy conservation and irreversibility of these processes as they imply small amounts of dissipation of free energy and thus production of entropy.

2.2 Are HRUs and landscape organization resulting from co-evolution?

Spatial organization in the critical zone itself manifests across a wide range of scales through different fingerprints, affecting both gradients and resistances controlling terrestrial water and energy flows (and stocks). The persistence of topographic gradients is the most obvious form of spatial organization, which implies the existence of catchments with perhaps the strongest and best-known implications for terrestrial water flows. A spatial correlation in, for instance, soil hydraulic properties (Zimmermann et al., 2008) reflects spatially organized storage of soil water and spatially organized capillary rise against gravity within a given soil (Western et al., 2004; Brocca et al., 2007; Blume et al., 2009; Zehe et al., 2010b). The soil catena reflects organized formation of different soil types along the gradient driving lateral hillslope-scale water fluxes (Milne, 1936), which implies partly deterministic patterns of infiltration and overland flow formation.

The omnipresence of networks of preferential flow paths is often regarded as *the* prime example of spatial organization (Bejan et al., 2008), because, independently from their genesis, they exhibit similar topological and functional characteristics. Topologically connected, network-like structures such as surface and subsurface preferential flow paths (surface rills, macropores, pipes), or vegetation and near surface atmospheric turbulent structures, create a strong anisotropy in flow resistances controlling mass and energy flows by strongly reducing dissipative losses within the network. This implies accelerated fluxes at a given driving gradient either of liquid water during rainfall driven conditions or of latent heat and water vapor during radiation driven conditions, thereby an increased power in associated energy fluxes (Kleidon et al., 2013). This in turn implies either an increased free energy export from the hillslope/catchment control volume or an increased depletion of internal driving gradients and thus a faster relaxation of the system back towards local thermodynamic equilibrium (Kleidon et al., 2013; Zehe et al., 2013). This common functionality might explain the dominance of rapid flow in different forms of connected network-like flow paths across many scales: locally in vertical macropores (Beven and Germann, 1982, 2013), in hillslope-scale lateral surface rills or subsurface pipe networks (Bull and Kirkby, 1997; Parkner et al., 2007; Weiler and McDonnell, 2007; van Schaik et al., 2008; Wienhöfer et al., 2009) or in catchment-scale and even continental-scale river networks (Howard, 1990).

We think that the idea of HRUs essentially implies that landscape evolution creates spatial organization, which is reflected in similar hydrological behavior of landscape entities/control volumes with similar structure. The underlying reason might be a co-evolution of distinct natural communities, landscape characteristics *and* suitable management practices (Watt et al., 1947; Winter, 2001; Schröder, 2006; Schaefli et al., 2011; Jefferson et al., 2010; Troch et al., 2013), because apparent spatial organization in a catchment has been formed in response to past hydro-climatic and management regimes (Phillips, 2006; Savenije, 2010). Locations at the hilltop, i.e., the sediment source area, the mid slope, i.e., sediment transport zone, or the hillfoot/riparian zone sediment deposit area have experienced distinctly different weathering processes and micro-climatic conditions causing formation of typical soil profiles with distinct soil texture and matrix properties in different horizons. This might, depending on hillslope position and aspect, imply formation of distinct niches with respect to water, nutrient, and sunlight availability and thus “filters” to (a) select distinct natural communities of vegetation (Tietjen et al., 2010) and soil macro fauna (Keddy, 1992; Poff, 1997; Schröder, 2006), and (b) constrain the appropriate forms of land use (Savenije, 2010). This in turn implies a similar ensemble with respect to formation of biotic flow networks (burrow systems of ants, earthworms, moles, and voles, as well as root systems), which feeds back on flows of water, mass, and thermal energy (Tietjen et al., 2009), which in turn create feedbacks on the vegetation habitat (Tietjen et al., 2010).

In this sense, we propose that structural similarity of, for instance, hillslopes might imply that past process patterns and human “disturbances” have been similar (Watt et al., 1947; Schröder, 2006). If we accept this, it seems logical that structurally similar landscape entities that are exposed to a similar management regime also exert at present similar controls on hydrological dynamics at different scales.

2.3 From response units to a hierarchy of functional units

Based on Eq. (1) and the associated mass and energy balances, we define functional units as classes of landscape entities/control volumes with similar terrestrial controls on the pair of gradient and resistance fields (referred to as $(\nabla\Phi, R)$ in the following) controlling either land surface energy exchange (thereby water vapor release) or different forms of stream flow generation (thereby liquid water release). This definition is consistent with the HRU definition as well as with the original idea of representative elementary watersheds (REWs) of Reggiani et al. (1998), as hydrologically homogeneous control volumes. At the same time, this definition offers a broader perspective, because the extent of functionally similar control volumes might (likely) be different for the different forms of water release (as already suggested by Vogel and Roth, 2003). We propose that homogeneity with respect to the terrestrial controls of the pair $(\nabla\Phi, R)$ might emerge at three different scales, namely (1) at the small field scale with respect to $(\nabla\Phi, R)$ controlling the

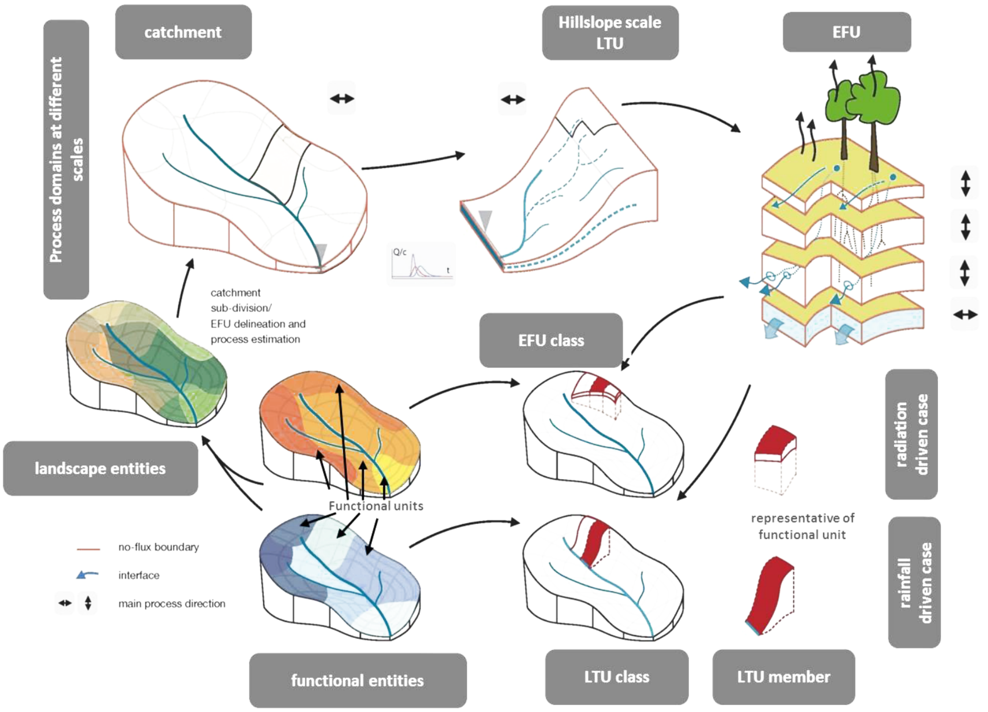

Figure 1. Catchment functioning reflecting context-dependent controls of different elementary functional units (EFUs) or lateral topological units (LTUs). Members of the same EFU class exert similar terrestrial controls on the surface energy balance (when in similar states and exposed to similar radiation/rainfall forcing). EFUs thus control functional similarity during radiation-driven conditions acting in parallel; class members could be ideally represented by the same parameter set related to the energy balance and vertical water flows. Members of the same LTU class exert similar terrestrial controls on rainfall runoff generation as the embedded EFUs are interlinked by lateral, gravity-driven water flows. Hillslope-scale LTUs control functional similarity; members of classes could be ideally represented by the same parameter set characterizing lateral flows and EFU-scale parameters.

land surface energy balance, (2) at the hillslope scale with respect to ($\nabla\Phi$, R) controlling rainfall-runoff transformation, and (3) at the headwater/subcatchment scale with respect to ($\nabla\Phi$, R) controlling groundwater storage and release. As a consequence, we propose the existence of three specific functional units (specialized HRUs) for a specific form of “water release”, which operate at the three different scales (Fig. 1):

- Field-scale elementary functional units (EFUs) of the same class are expected to function similarly with respect to the land surface energy balance and ET. They dominate catchment functioning during radiation-driven conditions, acting vertically and thus in parallel. Members of different EFU classes are characterized by similarity of the terrestrial properties controlling the radiation balance, the Bowen ratio, ET and root water uptake, and upward flows of capillary water in the soil matrix (Fig. 2, Table 2).

- Hillslope-scale lateral topological units (LTUs) of the same class are expected to function similarly with respect to runoff formation during rainfall-driven conditions. They release water during and after rainfall events due to activated, topologically connected flow paths which dominate free water fluxes either at the surface, in subsurface lateral drainage networks, or at the bedrock interface or through fractures to the aquifer. Members of the same LTU class thus share the same dominant runoff mechanism, and consist of the same organized sequence of EFUs from the hill crest to the stream, which are likely interconnected by the same type of lateral (preferential) flow paths (Fig. 2, Table 2).

- Sub-catchment-scale hydro-geomorphic units (HGUs) of the same class function similarly with respect to groundwater storage and release. HGU classes are determined by the hydro-geological and geomorphic setting of subcatchments. This determines the starting point for morphological processes, thereby constraining the set of hillslope forms, as well as parent rock for soil formation (Fig. 2, Table 2).

Overall, this idea implies that operative dominance of these functional units is not static, but depends on the prevailing forcing conditions – either rainfall driven or radiation driven. These conditions determine the degrees of freedom for the catchment to release water either to

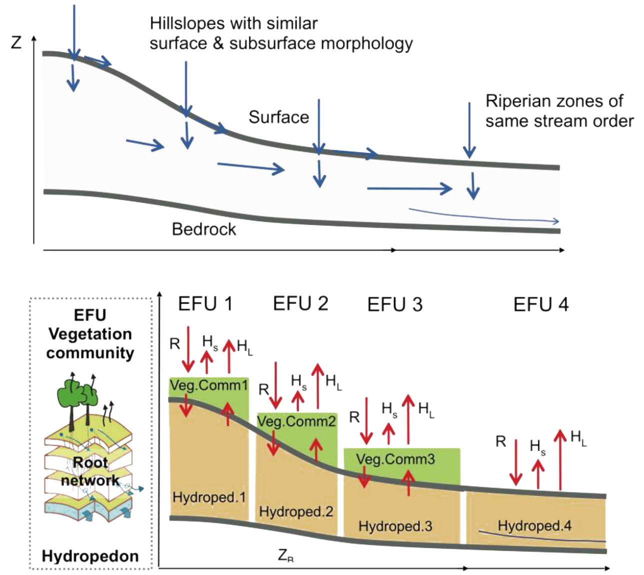

Figure 2. Scheme of lateral topological units and embedded elementary functional units controlling rainfall runoff response and land atmosphere energy exchange.

the atmosphere or as event runoff alongside the different driving gradients, different associated preferential flow paths that get potentially activated, and different forms of water storage depletion. Before we further explain how the proposed hierarchy might facilitate a representative experimentalcharacterization of intermediate-scale catchments, it is necessary to reflect on equifinality (Beven and Freer, 2001) as an inherence of hydrological dynamics.

2.4 Equifinality as inherent in our governing equations and options for its reduction

Equation (1) is inherently subject to equifinality as several combinations of gradients and resistances yield the same flux (e.g., an increase in bedrock slope can be compensated by decreasing subsurface hydraulic conductivity to yield the same flux). This might frequently be the case in hydrological systems as the quasi-static controls on gradients driving lateral flows of free water during rainfall-runoff transformation are largely independent of those that determine the flow resistance. In line with Bardossy (2007) we suggest that the equifinality in Eq. (1) can partly be reduced by collecting information that characterizes at least two of the three variables: either q (or a proxy thereof) and terrestrial controls on R, or q and terrestrial controls on $\nabla\Phi$, or terrestrial controls on $\nabla\Phi$ and R. This option has clear implications for:

- A feasible experimental design to characterize intermediate-scale catchments, which should rely on characterizing the outlined pairs (if possible) in replicate members of candidate functional units along the proposed hierarchy;
- The structural adequacy of models, which should be thermodynamically consistent (as already called for by Reggiani et al., 1998) and thus able to disentangle the driving gradients and resistances controlling hydrological fluxes. This allows, for instance, constraining the set of feasible behavioral subsurface flow resistances by incorporating available information on the corresponding gradients driving lateral flows (e.g., bedrock topography).

Current technology allows in principle the characterization of the terrestrial controls of all hydrologically relevant gradients, and even bedrock topography may be approximated using geophysical imaging techniques. Fingerprints of lateral subsurface fluxes and resistances (including fingerprints of preferential flow paths) may be retrieved from natural and artificial tracers. Also ET patterns can be estimated by new remote sensing techniques coupled with high-resolution soil–vegetation–atmosphere transfer (SVAT) modeling. However, a combination of these techniques with soil physical methods, to characterize resistance terms, or sap flow to estimate local transpiration fluxes, is hampered by well-known scale issues and the high amount of labor, and is thus only feasible to a limited extent. We thus suggest clustering of these observations in replicate members of EFU or LTU classes, mainly to explore whether their main structural and functional characteristics can indeed be characterized in an exemplary manner. If this were true, it would imply that behavioral model parameters characterizing structure and functionality of EFUs or LTUs were indeed transferable among all members of the same class.

3 Implications for experimental characterization of intermediate-scale catchments

The idea of HRU or specific functional units implies that their typical dynamic behavior might be grasped by thoroughly characterizing the structural setup and functionality of a subset of only a few members of each class. Up to now, a large set of HRU separation methods has been suggested, such as (an exhaustive review being beyond the scope of this paper):

- Topographic indicators to support geomorphology-based predictive mapping of soil thickness (Pelletier and Rasmussen, 2009), soil erosion processes (Märker et al., 2011), and other soil properties (Behrens et al., 2010), or
- Explanations of the variability of base flow response based on climatic, soil and land use characteristics (Santhi et al., 2008; Haberlandt et al., 2001), or even
- Schemes to predict the locally dominating runoff processes based on soil, topography, land use, and

Table 2. Hierarchy of proposed functional classification scheme, controlled form of water release, candidate descriptors, dominant preferential flow path, and hydrological context of dominance.

Hierarchy level	Similarity	Descriptors	Preferential flow path	Dominance
HGU (catchment scale)	Base flow, groundwater storage	Parent rock for soil formation, aquifer, geomorphology	River network	Permanent, long term
LTU (hillslope scale)	Rainfall runoff transformation, free water storage	Potential energy differences: surface & bedrock topography, catena, aspect	Vertical macropore, lateral pipe or rill network	Rainfall-driven conditions
EFU (field scale)	Land surface energy exchange/ET, capillary soil water supply	Slope position and aspect, land use, soil type	Vegetation	Radiation-driven conditions

small-scale experiments for agricultural land (Naef et al., 2002; Schmocker-Fackel et al., 2007).

A rigorous experimental test of whether HRUs exist in the landscape has, however, never been carried out. A major obstacle to implementing such an experimental test, or more precisely to searching for the proposed hierarchy of functional units, is to balance the need for exhaustive characterization of the triple of (q, $\nabla\Phi$, R) within class members of functional units with the need to conduct replicate experiments and monitoring to detect typical functional and structural characteristics among class members. The null hypothesis, for example for EFUs, is that their class members belong to the same ensemble with respect to the interplay of the energy balance (including ET), root water uptake, and capillary soil water dynamics. This implies that mean and spatiotemporal variability of, for instance, sap flow, soil moisture, and surface and soil temperature dynamics observed within replicates should be identical within the confidence limits, and significantly differ from the corresponding observations obtained in members of other EFU classes. However, to ensure an acceptable significance level of such a test of concept one cannot exclusively rely on observations, because the sample sizes, N, within EFU class members are likely to be small (and the confidence limits of the mean decrease with $N^{-1/2}$). This exercise must thus be essentially combined with a test of whether behavioral model parameter *sets* are transferable among class members of functional units at the same hierarchy level.

3.1 How to characterize EFUs and their structure and functionality?

3.1.1 Controls and characteristics of EFUs

We hypothesize that similarity with respect to the surface energy balance and ET emerges at the EFU/field scale ($1000\,\mathrm{m}^2$) due to emerging homogeneity with respect to the terrestrial controls on the radiation balance, root water uptake and capillary water storage/upward capillary rise. This is because the covariance lengths of the governing soil hydraulic parameters, soil moisture, and controlling vegetation are in the order of 1–10 m (Zimmermann et al., 2008; Zehe et al., 2010b; Gerrits et al., 2007). We further suggest that lateral variability of soil water potential at a given depth is during energy-driven conditions rather small at this scale. This is supported by the observed stability of ranks and absolute mean differences among 80 soil moisture sensors Zehe et al. (2010b) clustered at a forested and grassland site. The reported persistence of these differences at a scale extent of 10 by 10 m might reflect small-scale heterogeneity of soil texture, but not necessarily differences in driving potentials. This is because the persistence of differences can be explained by absence of lateral soil water flows, which in turn may be due to absence of a lateral gradient in soil water potential. The latter implies that a vertical 1-D treatment of soil water flow (as proposed in Sect. 4.2) is still appropriate at this scale.

Our first guess predictors for detecting candidate EFUs in a given geological setting are thus land use and management practice, location within the catena, and hillslope aspect (Fig. 2, Table 2). These factors determine exposure to global radiation, surface albedo, and either the age spectrum and species composition of trees in forest areas or surface preparation and selection of crops in agricultural areas (with a certain plant albedo).

3.1.2 Characterization of the energy balance and gradients and resistances at the EFU-scale

For EFU detection and characterization we propose combined observations of global radiation and the albedo ($\nabla\Phi$), sap flow (relates to q) within trees species of representative age stages, air temperature and humidity (relate to $\nabla\Phi$) clustered along the catena at upslope, midslope, downslope locations and in the riparian zone. This should be completed with observations of soil water characteristics at the same sites (with all the known difficulties) to characterize soil hydraulic conductivity (relates to R during capillary rise) and the soil water retention curve driving upward capillary water flow (relates to $\nabla\Phi$). We propose a combination of in situ observations of soil moisture and matric potentials in the field (for inverse modeling and soil landscape modeling), permeameter measurements and undisturbed soil cores to be analyzed in the lab. Comparison of inverted hydraulic parameter sets with those derived from soil samples quantifies the effect of activated preferential flow paths, as the former jointly represent flow in both domains (Troch et al., 1993; Hopp and McDonnell, 2011).

As some networks of preferential flow paths are created by biota such as earthworms, ants, and rodents (Lavelle et al., 2006; Meysman et al., 2006), an ecological survey of the abundance and number of individuals of soil ecosystem engineers creating vertical and lateral preferential flow paths might yield helpful proxy information on density and depth of biotic macropores.

3.2 How to identify LTUs and characterize their structure and functionality?

3.2.1 Controls and characteristics of LTUs?

Class members of hillslope-scale LTUs are deemed to belong to the same ensemble with respect to controls of rainfall runoff behavior (note that we exclude homogeneity with respect to base flow production here). We propose that homogeneity with respect to the terrestrial controls on rainfall interception and the gradients driving vertical and lateral fluxes of free water emerges at this scale. This is because hillslopes are key elements organizing rainfall-runoff transformation in many intermediate-scale catchments (e.g., Troch et al., 2004; Berne et al., 2005), connecting areas of maximum potential energy located at the watershed boundary to local minima in potential energy located at the stream, which the latter marking a local minimum in potential energy. Hillslopes are already large enough to be distinguished based on typical spatial patterns characterizing their flow path morphology (confluent, parallel, divergent), their hydro-pedology based on the soil catena (Milne, 1936) and permeability of the parent rock including dip direction and slope of facies and optionally fractures.

Then again, hillslopes are smaller than the length scales of meso-scale and even of most micro-scale atmospheric structures (including convective rainfall cells); spatial variability of the atmospheric forcing within the hillslope is thus controlled by slope topography, aspect, and land use. The fact that rainfall runoff in different hydro-climates may be successfully simulated using model structures that rely on several typical hillslopes as building blocks (Güntner, 2002; Zehe et al., 2005, 2013; Jackisch et al., 2014) is another strong argument that homogeneity with respect to rainfall-runoff transformation emerges at the hillslope scale.

We propose that within a given hydro-geological and geomorphic setting, a similar surface and bedrock topography and morphology alongside a similar land use are first-order determinants for LTU classes (Fig. 2, Table 2). These factors determine the ensemble for interception and infiltration, as well as the steepness of the water level/potential energy gradient that might drive lateral flows and the conditions for sediment redistribution and formation of the soil catena.

3.2.2 Characterization of rainfall-runoff transformation, gradients and resistances at the LTU scale

As neither flow at the bedrock interface nor in lateral pipe networks is directly observable, we still struggle to understand how, when and why hillslopes connect to the stream. In recent years promising new investigation techniques have been proposed to add bits and pieces to this puzzle; for instance, distributed temperature surveys (DTSs) of groundwater inflow locations along streams (e.g., Selker et al., 2006; Westhoff et al., 2007) or thermal infrared imagery of saturated area dynamics (e.g., Pfister et al., 2010; Schuetz and Weiler, 2011). Source areas of runoff onset and cessation in the hillslope, riparian zone, stream continuum might be characterized using biological tracers (Pfister et al., 2009), occasionally with radon as a tracer of groundwater input and extensive observation networks (e.g., Jencso et al., 2010; Tromp van Meerveld and McDonnell, 2006).

Bedrock topography, as key control on gradients driving lateral flow, may be furthermore approximately characterized by geophysical imaging techniques such as electric resistivity tomography (ERT, e.g., Graeff et al., 2009) or ground penetrating radar (GPR). These techniques are, however, laborious and need to be validated with auger profiles, because even joint geophysical inversions can be non-unique (e.g., Binley et al., 2002; Paasche and Tronicke, 2007). Time-lapse GPR using a shielded antenna is furthermore promising for in situ observation of shallow subsurface hydrological processes. Up to now such surface-based techniques are rarely used for monitoring purposes. Because of the high demands on data quality only a handful of successful examples is reported, which are mainly carried out in controlled environments such as sand boxes (e.g., Versteeg and Birken, 2001; Trinks et al., 2001; Truss et al., 2007; Haarder et al., 2011).

3.3 How to identify HGUs and to characterize their structure and functioning?

3.3.1 Controls and characteristics of HGUs

We expect homogeneity with respect to groundwater storage and release to emerge at the headwater or even subcatchment scale and to be largely determined by the hydrogeological setting, land use, and of course the climatic setting. The hydro-geological setting determines parent rock for soil formation, as well as the nature and the properties of the aquifer, while land use and climate largely determine groundwater recharge. HGUs should thus ideally have homogeneous geology, climate conditions and land use. As this rarely is the case in intermediate-scale catchments, there is a need to understand how homogeneous geologies and land uses as well as different mixtures thereof control groundwater storage and release.

3.3.2 Characterization of free water storage and release across scales and geologies

The majority of the related tracer-based investigations have been carried out in small, geologically homogenous, experimental catchments (Klaus and McDonnell, 2013). More recent work has begun to explore tracer signatures across scales, ranging from hillslopes to headwaters (e.g., Uchida et al., 2005; McGuire and McDonnell, 2006) to lower mesoscale ($\sim 200\,\mathrm{km}^2$) catchments. McGuire et al. (2007) showed for the Western Cascades in Oregon that mean transit time (MTT) was positively correlated to flow path length and negatively correlated to flow path gradient. Additionally Hrachowitz et al. (2009) reported for a set of 20 headwater catchments (1 to $35\,\mathrm{km}^2$) that MTT is strongly controlled by precipitation intensity and soil cover, drainage density and topographic wetness index. While geological factors have been omnipresent in MTT scaling studies, few investigations have been able to identify distinct geological differences across nested and neighboring catchments (e.g., Sayama et al., 2011). However, studies available today (e.g., Maloszewski et al., 1992; Dewalle et al., 1997; Viville et al., 2006; Tetzlaff et al., 2006, 2009; Heidbüchel et al., 2013) do not yet span a wide enough range of bedrock types where both flow and isotope tracer data are available to draw more general conclusions on how catchment bedrock conditions influence mixing, storage, and release across scales. Such studies should furthermore be completed by a characterization of the space/time variability of climate and land-use controls.

4 Implications for structurally adequate modeling

4.1 Reduce inherent equifinality by removing physical and structural biases

4.1.1 Thermodynamically consistent model equations

We already proposed that structurally adequate models for intermediate-scale catchments should be thermodynamically consistent to draw advantage from the structure of Eq. (1) by including available data on a pair out of the triple of flux, gradient, resistance (q, $\nabla\Phi$, R). This allows constraining of the set of feasible behavioral subsurface flow resistances by incorporating available information on bedrock topography at the hillslope scale, as well as soil water retention properties and proxies for macroporosity along the catena. As an exhaustive observation of these characteristics at the intermediate scale is out of reach, this option is feasible only if the structure and functionality of functional units may indeed be exemplarily characterized and the related behavioral, structural, and functional parameter sets are indeed transferable among members of the same EFU or LTU class.

Most conceptual models are not thermodynamically consistent because they merge driving gradients and resistances into effective descriptions (Westhoff and Zehe, 2013). Distributed physically based models employ thermodynamically consistent model equations; commonly the Darcy–Richards approach, the convection dispersion approach, and approximations of the Saint-Venant equations. In principle, they allow consistent predictions of internal dynamics and input–output behavior, including non-Gaussian transport, based on different conceptualizations of preferential flow up to the headwater scale, as recently shown by, for example, Gassman et al. (2013). Nevertheless, a full 3-D physically based model might not be a “perfect model” for intermediate-scale catchments, either when defining perfection on the basis of a balance of complexity and parsimony or with respect to straightforward accessibility of structural model errors (Reusser et al., 2011; Reusser and Zehe, 2011).

4.1.2 Disentangling matrix fluxes and rapid fluxes in connected networks

Model structural adequacy also requires, in our opinion, separate treatment of fluxes in matrix/continuum elements and connected network-like structures. This should be addressed for vegetation controlling transpiration, for flow in the river network, and in particular for subsurface vertical and lateral preferential flows, for several good reasons. First, because matrix flow and preferential flow sustain different forms of water release, they are dominated by different forces (either capillary forces or gravity) and deplete different gradients in free energy, as explained above. Second, with the soil matrix and preferential flow paths acting as independent factors that control subsurface flow resistances, they are independent sources of equifinality (e.g., Binley and Beven, 2003; Wienhöfer and Zehe, 2014). Preferential flow networks with different topological and hydraulic properties may result in the same control volume resistance and thus match observed flow and transport equally well, even if all other model parameters are kept constant (Wienhöfer and Zehe, 2014). Separate treatment of matrix flow as well as vertical and lateral preferential flow allows constraining of the degrees of freedom in both flow domains independently, using different appropriate sources of information and genetic knowledge about the differences in their origin.

An exhaustive overview of the wide range of methods that have been proposed for representing subsurface flow in vertical and lateral preferential flow paths is beyond our scope; Šimůnek et al. (2003), Gerke (2006) and Köhne et al. (2009), among others, have published such overviews. In line with studies of Vogel et al. (2006), Sander and Gerke (2009), and Klaus and Zehe (2011), we prefer a spatially explicit representation as vertical and lateral connected flow paths.

This approach preserves the flow path topology (Wienhöfer and Zehe, 2014) and may be parameterized based on observable field data or on estimates from species distribution models for ecosystem engineers (Schröder, 2008; Schneider and Schröder, 2002). Such an explicit approach furthermore allows testing of thermodynamic optimality principles, which allow for a priori optimization of the resistance field at a given gradient (Porada et al., 2011). This implies the possibility of independent predictions based on optimized model structures and preferential flow networks (compare to Sect. 4.3).

4.2 What is a perfect (and yet thermodynamically consistent) model?

"Perfection is achieved, not when there is nothing more to add, but when there is nothing left to be taken away". In line with this *bon mot* of Antoine de Saint-Exupéry, we regard a model as perfect if it balances necessary complexity with the greatest possible parsimony. Although thermodynamic consistency of equations and separate treatment of matrix and preferential flow are not negotiable, we think that simplicity can be achieved for instance by stating clear hypotheses on (a) how spatial organization creates anisotropy in dominant terrestrial water and energy flows (thereby reducing dimensionality of the governing equation set), or (b) how to account for preferential flow paths and how to couple fast and slow flow domains, or (c) how to conceptualize driving gradients in a smart and unbiased manner.

4.2.1 Pioneering research and models to balance necessary complexity with parsimony

The Representative Elementary Watershed (REW) approach proposed by Reggiani et al. (1998) is certainly pioneering in proposing a simplified but thermodynamically consistent treatment of the mass, energy, and momentum balance of hydrologically homogeneous control volumes (named REWs). Reggiani et al. (1998, 1999) derived the set of balance equations for the REW and subcontrol volumes/process domains (e.g., the unsaturated and saturated flow domains, characteristic areas where either Hortonian or Dunne's overland flow dominate) using thermodynamic consistent averaging (Reggiani et al., 1998, 1999; Reggiani and Schellekens, 2003; Reggiani and Rientjes, 2005). The related parameters and state variables are, thus, to be regarded as effective representations of point scale state variables and parameters (Zehe et al., 2006; Lee et al., 2007; Mou et al., 2008). Beven (2006) identified the assessment of suitable closure relations to characterize exchange flows of mass, energy, and momentum as the cardinal problem when applying the REW approach to real catchments. And there has been considerable progress in this respect: REWASH developed by Reggiani and Rientjes (2005) has been successfully applied to the Geer catchment in Belgium and to the Donga basin in Benin by Varado et al. (2006). Zhang et al. (2006) introduced a macropore flow domain into the REWASH model, which considerably improved its performance when applied to the Attert basin. In particular they were able to simultaneously reproduce stream flow and distributed observations of groundwater.

However, all the listed applications of the REW approach up to now treat sub catchments and REWs as synonymous and flow within the control volumes in a spatially averaged zero-dimensional manner. This is problematic as it implies averaging across different ensembles – for instance soil types – and with respect to the local equilibrium assumption. Furthermore, it is exactly the deviation from the spatial average compared to the uniform distribution what makes up spatial organization. Thus, the REW approach is in our opinion over-simplified with respect to how it represents different forms of hillslope scale spatial organization and thus eventually with respect to how it reduces equifinality in the manner specified above.

The hillslope storage Boussinesq (HSB) model proposed by Troch et al. (2004) is another pioneering work, based on an analytical solution of the linearized Boussinesq equation that describes discharge from a free unconfined aquifer that develops over impermeable bedrock. The HSB model is tailored for hilly landscapes with shallow, permeable, weakly heterogeneous soils, where subsurface storm flow and saturated excess overland flow dominate runoff generation (Hilberts et al., 2004, 2005; Troch et al., 2004; Berne et al., 2005). Although treatment of hillslope scale spatial variability of infiltration is a challenge, this concept is valuable in the sense that rainfall-runoff transformation is dominated by lateral fluxes of free non-capillary water and a simplified but unbiased treatment of this process.

A simplified but unbiased accounting for terrestrial controls on driving gradients does not necessarily imply a switch to models based on coupled partial differential equations. TOPMODEL (Beven and Kirkby, 1979), WASA (Güntner, 2002), and mHm (Samaniego et al., 2010) are based on smart but explicit conceptualization of how landscape characteristics in different hydro-climates determine the gradients and resistances controlling the dominant runoff formation process. WASA is tailored for semiarid landscapes where Hortonian overland flow dominates and the catena is the dominant landscape element (Jackisch et al., 2014). The TOPMODEL assumptions, which cumulate into the idea that points with a similar topographic index act hydrologically similarly (Beven and Freer, 2001b), are likely fulfilled in a humid climate with shallow, highly permeable soils over impermeable bedrock. Although we appreciate the progress achieved with TOPMODEL (Beven and Kirkby, 1979) and dynamic TOPMODEL (Beven and Freer, 2001b) – as perhaps the most famous and smartest conceptualization of landscape controls on liquid water release (rainfall runoff and base flow production) – we think that it is nonetheless too simple for catchments that are dominated by other runoff generation mechanisms, as well as in terms of land-surface energy exchange and capillarity-dominated flow during radiation-driven conditions. However, it would be unfair only to blame TOPMODEL as being too simple in terms of predictions of land-surface energy exchange: most hydrological and land-surface models produce severe errors in this respect, especially with respect to the influence of vegetation. Another error source is shallow turbulence parameterization, which is in most atmospheric based models on Monin–Obukhov similarity and related stability functions. The underlying key assumptions – horizontal homogeneity and constant turbulent fluxes near the ground – are, however, questionable at intermediate scales, especially in the case of a rugged topography.

4.2.2 Suggestion of a simple but structurally adequate modeling framework: the CAOS model

The CAOS (Catchment as Organized Systems) model simulates water, tracer, and heat dynamics based on thermodynamically consistent equations and disentangles matrix and preferential flow. Our proposition to achieve parsimony is to represent only the dominant matrix and preferential flow processes at the EFU, hillslope, and catchment levels in a coupled but 1-D manner. We further propose that flow in network-like structures dominates over matrix flow during rainfall-driven conditions. The CAOS model consists of hierarchical objects (Fig. 3) with the catchment object on top, followed by hillslope and riparian zone objects. The least model entities are not REWs but EFUs, which control vertical flows of land-surface energy exchange and ET (based on the Penman–Monteith approach) and related vertical flows of upward capillary rise and soil heat during radiation-driven conditions or downward gravity-driven preferential flow during rainfall-driven conditions. During radiation-driven conditions we use the Darcy–Richards equation, which, although often criticized, is still the best concept to describe capillary-driven water flows. Flow in the macropore domain during rainfall-driven conditions is represented either through a kinematic wave equation or via a stochastic approach. As motivated by Davies and Beven (2012), the latter consists in treating water flows during rainfall-driven conditions by means of a space–time domain random walk of water particles. Diffusive model parameters may be estimated based on soil water characteristics, while the probability density function of advective flow velocities in preferential pathways is retrieved from tracer travel depth or travel time distributions. Related macropore densities and depth may be estimated from dye staining, time lapse GPR, or data on the abundance of ecosystem engineers. Water beyond saturation is directed to either the macropore domain or the Rapid Subsurface Flow object, which laterally connects EFUs along the downslope driving gradient. The lower boundary condition is free drainage which connects to the Slow Groundwater Flow object.

Lateral exchange between EFU objects during rainfall runoff is treated in separate hillslope-scale network domains representing either overland flow in rills or subsurface lateral flow. Flow within these networks is modeled with the diffusion wave or the Darcy–Weisbach equation respectively. Motivated by the experimental findings of van Schaik et al. (2008), van Schaik (2009) and by unpublished experimental findings of an irrigation experiment outlined in Sect. 5.1.1, we neglect exfiltration from the lateral flow domains into the surrounding matrix/EFU objects. The slow groundwater domains account for base flow production through a diffusion wave equation. It receives its water from the lower boundary of the matrix domain and the rapid subsurface flow object. Groundwater flow on the hillslope is assumed to be homogeneous perpendicular to the line of steepest descent. The stream domain is also represented as a network. It receives its water from the Rapid Subsurface Flow and Slow Groundwater Flow objects of all connected hillslopes. Flow is described with the kinematic wave equation. Each of the model objects has a transport module based on the advection–dispersion equation, including a decay term to account for the transport of solutes, isotopes or thermal energy. Adaptive time stepping and the same explicit/implicit Crank–Nicolson scheme as in the water flow solvers are used.

An example of the overall model output is given in Fig. 3. The restriction to multi-1-D representations and of the EFU size to be approximately 1000 m^2 and applying the "θ-based" version of the Richards equation reduces the computation time significantly. With respect to model complexity, the CAOS model concept is on the one hand steps beyond the REW concept (Reggiani et al., 2005; Lee et al., 2007) as it avoids averaging across landscape components of different function and hence allows closure of the mass, momentum, and energy balance in a spatially resolved manner. On the other hand, the model is clearly simpler than fully distributed, physically based models such as HydroGeoSphere, HYDRUS 3D and CATFLOW.

4.3 Thermodynamic consistency to test thermodynamic optimality

4.3.1 Organizing principles – a possible link between catchment structure and functioning

Several authors suggest that water flow in catchments and catchment structure is in accordance with different candidate optimality principles that characterize the associated energy conversions and related thermodynamic limitations (Phillips, 2006; Paik and Kumar, 2010; Phillips, 2010). Woldenberg (1969) showed that basic scaling relationships of river basins can be derived from optimality assumptions regarding stream power. Similarly, Howard (1990) described optimal drainage networks from the perspective that these minimize the total stream power. Rinaldo et al. (1992) explain river networks as "least energy structures" minimizing

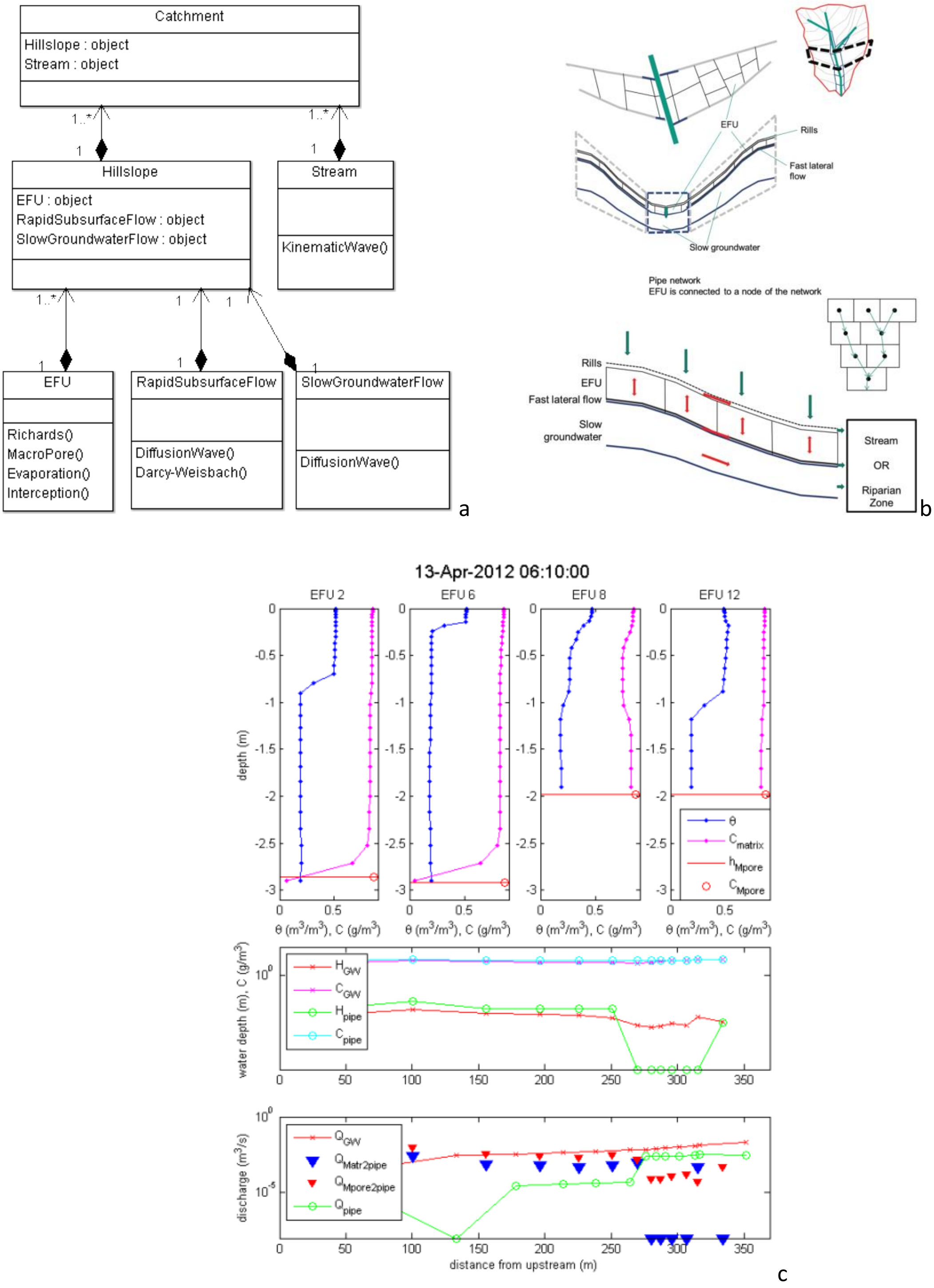

Figure 3. (a) Simplified UML diagram of the current CAOS model structure. Each object either has child objects or solves 1-D flux equations. **(b)** Sketch of the physical model elements. **(c)** Exemplary visualization of model states and output: top panels show EFU soil moisture profiles and tracer concentrations, middle panel shows water levels and tracer concentration in fast and slow lateral flow domains, lower panel shows discharge from soil matrix and macropores into pipes as well as along the lateral flow domains. Numerical solutions have mass relative balance errors of order 0.001 to 0.01.

local energy dissipation, and based on this they reproduced observed fractal characteristics of river networks.

Related to these energetic minimization principles, the literature debates several principles that seem to state exactly the opposite (Paik and Kumar, 2010): that systems organize themselves to maximize steady state power (MAXP proposed by Lotka (1922)), steady state net reduction of free energy (MRE – Zehe et al., 2010, 2013), or steady state maximized entropy production (MEP – Paltridge, 1979) associated with environmental flows. The MEP hypothesis has been corroborated within studies that allowed (a) successful predictions of states of planetary atmospheres (Lorenz et al., 2001), (b) identification of parameters of general circulation models (Kleidon et al., 2006), or (c) identification of hydrological model parameters to estimate the annual water balances of the 35 largest basins on earth (Porada et al., 2011). Kleidon et al. (2013) recently explored whether the formation of connected river networks is in accordance with MAXP and thus whether "free" energy transfer to sediment flows is maximized. What they showed is that the depletion of topographic gradients by sediment transport is linked to a minimization in frictional dissipation in streamflow, so that maximization and minimization approaches may not necessarily contradict each other.

We thus suggest that these outlined maximization and minimization principles are largely two sides of the same coin, because local minimization of frictional dissipation of kinetic energy increases the flow's ability to transport matter against the driving macroscale gradient and thus to deplete it.

4.3.2 Promising findings and the need for stronger tests

These outlined organizing principles allow for a priori optimization of the resistance field at a given gradient (Porada et al., 2011) with respect to an objective function. This implies the possibility of independent predictions either using an optimized bulk resistance (Westhoff et al., 2014) or based on an optimized density of vertical and lateral macropores (Zehe et al., 2013; Kleidon et al., 2013). If conclusive, this might be seen as an argument that at least the potential natural state of a catchment as open terrestrial system functions in accordance with such a principle.

Zehe et al. (2013) provided evidence that the spatially organized pattern of soils and macropores in the Weiherbach, reflecting past erosion processes (Zehe and Blöschl, 2004) and habitat preference of anecic earthworms (van Schaik et al., 2014), is superior to other tested arrangements with respect to long-term reduction of free energy of soil water. This implies that the true system configuration operates closer to local thermodynamic equilibrium (LTE) than the other configurations. They showed furthermore that an uncalibrated 1.5-year simulation of rainfall-runoff transformation based on an apparent thermodynamic optimum in the surface density of macropores, which maximized free energy reduction during rainfall runoff processes (thereby minimizing system time to recover back to LTE), performed as well as the best model setup calibrated based on rainfall runoff data. It seems that in this old agricultural landscape, the slow co-evolution of landforms, soil catena formed by erosion, and macropore patterns to a system architecture far from thermodynamic equilibrium implies that the system dynamics, however, operates close to local thermodynamic equilibrium, except for a few extreme events.

The same study by Zehe et al. (2013) revealed that the relatively young landscape in Malalcahuello catchment in the Chilean Andes, close to the Volcano Longymay, operates close to a steady state in the potential energy of soil water. A model structure assuming that gains in potential energy due to infiltration into these highly permeable volcanic ash soils are in the long term compensated by potential energy export by means of subsurface storm flow allowed an uncalibrated prediction of rainfall runoff within an Nash Sutcliffe efficiency (NSE) of 0.65. Finally, a parsimonious model for the land-surface energy exchange based on maximum power and Carnot efficiency by Kleidon and Renner (2013a, b) performed well, without calibration, against flux tower data at three sites with different land use and at the global scale against ERA 40 reanalysis data. This implies that turbulence in the convective boundary layer, which forms at a timescale of 10–20 min, is structured such that sensible heat fluxes operate close to the upper limit determined by Carnot efficiency.

We conclude that a thermodynamic perspective is very helpful for explaining the operative advantage of organized preferential flow structures: push it to the limit and minimum time for recovery. In case structures establish fast compared to characteristic time of mass and energy flows as in the boundary layer, they push the system to operate at its (Carnot) limit. In case organized structures result from a very slow co-evolution, as in the Weiherbach, they minimize time of the system to recover back to LTE. However, we acknowledge that (a) the validity and the practical value of thermodynamic optimality are still debated (see also discussion of this paper in HESSD) and (b) that the reported promising findings might be just a matter of coincidence. A test of concept based on successful uncalibrated predictions relies implicitly on the assumption that the model is "closed", i.e., is an acceptable representation of the system accounting for all relevant degrees of freedom and of the feedbacks between processes that form structures and their impact on water and energy flows. As none of the reported model studies is closed in this sense, there is a strong need to define rigorous model and real world experiments to test how far thermodynamic optimality applies.

5 Conclusions and outlook

The presented strategy for improving our quantitative understanding of how spatial organization controls storage and release of water and energy in intermediate-scale catchments has been driving joint research within the CAOS project for the last 2.5 years. Key objectives of the CAOS project are to test our three main propositions: on (a) a scale hierarchy of functional units and a strategy for their characterization, (b) requirements to be met by structurally adequate models, and (c) the search for organizing principles linking catchment structure and functioning. The area of focus is the Attert hydrological observatory basin in Luxembourg, which has been operated in since 1994 by the CRP–Gabriel Lippmann (e.g., Pfister et al., 2009, 2010; Martínez-Carreras et al., 2012). It consists of nine nested subcatchments that have homogeneous and mixed geologies ranging from schists to marl, sandstone and limestone, different land uses and a semi-oceanic climate.

5.1 Brief outlook on the ongoing proof of concept

5.1.1 Experimental design

In line with the hypotheses and ideas proposed in Sect. 3 for an experimental test of the HRU concept, 46 candidate EFUs in two candidate LTUs have been instrumented since 2011 with automated sensor clusters (SCs). A single SC collects data on rainfall ($N = 5$), air temperature, relative humidity, and wind speed, global radiation; soil moisture profiles ($N = 10$), electric conductivity ($N = 10$), and soil temperature ($N = 10$); matric potential ($N = 10$), water levels ($N = 4$) to observe groundwater and stream water levels, and five sap flow ($N = 4$). 23 sensor clusters are located within candidate EFUs in the schist area, of which 6 are along north facing slopes and 10 along south facing slopes, 7 units are situated close to a stream, and we included 16 forest and 7 pasture sites. Within the sandstone and marl areas 12 and 11 EFUs have been instrumented, respectively. This has been combined with an ecological survey of soil ecosystem engineers in combination with bromide profiles and dye staining. We sampled different earthworm species (in total 18 were found in the Attert catchment) and small rodents in a randomly stratified design at 117 locations (including the sensor cluster sites if possible), considering the gradients of different habitat factors covering the entire catchment. These data may serve as the basis for models predicting the spatiotemporal distribution of these species (Palm et al., 2013) and yield proxy information about preferential flow paths. To investigate the relevant subsurface structures and properties we have evaluated different geophysical techniques. The combination of ERT, GPR, and a few manual auger profiles has proved to provide important information on depth to bedrock and the depth of the weathered schist layer, and can be used to evaluate the consistency of the first-guess lead topologies and to estimate the downslope extent of EFUs within selected LTUs.

At the hillslope/LTU scale connectivity between hillslopes/riparian zones and streams has been characterized in detail for a tributary of the Colpach River in the Schist area of the Attert catchment. Within 50 m reaches we measured incremental discharge, including radon as a natural tracer to distinguish between young water and old water draining from the hillslopes into the streams. Additionally salt tracer experiments were performed to derive gains and losses for several headwater streams during different flow conditions. This was completed with hand-held Thermal infrared (TIR) and DTS temperature observations of the streams to identify localized inflow locations. At the event timescale we conducted a hillslope scale sprinkling experiment to explore the role of lateral subsurface flow in the near surface weathered schist layer and the feasibility of combining time lapsing GPR, time domain reflectometry (TDR) soil moisture profiling, and stable isotope profiling before and after the irrigation to jointly monitor subsurface flow processes within the upper 2–3 m.

The Attert observatory is also well suited to explore how homogeneous geologies and land use as well as different mixtures thereof control groundwater storage and release, as it provides natural tracer and rainfall runoff data for at least a decade for nine nested subcatchments (e.g., Pfister et al., 2002). Recent investigations focus on geological controls on isotopic signatures in baseflow and catchment dynamic storage (as per Sayama et al., 2011) and the spatial and temporal variance of storage capacities and dynamics, as well as of contributions from saturated and unsaturated zones. To this end we rely on the complementarities of multiple tracers (geochemicals, stable isotopes of O and H, tritium), hydrometric data and in situ observations and remote sensing of soil moisture.

Spatio-temporal variability of precipitation is of key importance for discriminating functional similarity and dissimilarity. It is characterized by merging operational rainfall radar data with rain gauge data as well as disdrometer data to characterize droplet sizes and vertical rain radar that have been installed within the Attert catchment at three meteosites. These data are combined: (a) by means of data assimilation into the soil–vegetation–atmosphere model system WRF-NOAH-MP (Skamarock et al., 2008; Schwitalla and Wulfmeyer, 2014) and (b) by a geo-statistical merging originally proposed by Ehret et al. (2008) for improving quantitative precipitation estimates. During radiation-driven conditions horizontally averaged sensible and latent heat fluxes are observed by means of a scintillometer and airborne thermal remote sensing that yields spatially highly resolved data on leaf temperature and soil surface temperature at different time slices. Spatial patterns of land cover and leaf area index are derived from Landsat and Modis satellite images to support EFU identification by means of pattern recognition.

5.1.2 Spatial transferability of parameters as genuine test of model structural adequacy

Transferability of model parameters of the CAOS model among members of the same functional unit class is a genuine test of whether the proposed hierarchy of functional

Table 3. Available observations and calibration parameters for CAOS model verification at different scale levels.

Forcing data	Observed parameters and parameter sets from lower level	Verification data	Parameters to be estimated
EFU verification			
Rain gauges from sensor clusters	Soil samples: soil water retention curves	Soil moisture: 3 profiles	Size of top soil layer
Meteorological data from sensor clusters	Auger information: soil layering ERT: depth to bedrock	Matrix potential: 1 profile	Van Genuchten parameters: small corrections to observed
3-D radar reflectivity from European network Micro rain radar Disdrometers	LAI	Sap flow: 5 trees	LAI: small corrections to observed
	Macropore density		Soil layers: small corrections to observed
Lateral flow network verification using sprinkling experiments			
Natural rainfall	Calibrated EFU parameters	Piezometric heads	Macropore domain: non-linearity and reservoir constant
Sprinkled water	GPR and ERT information: soil layering	Soil moisture: 16 profiles	Darcy–Weisbach: roughness, pipe diameter, number of parallel pipe networks
Isotopic signature of sprinkled water		Pre- and post-event isotope profiles	Diffusion wave: hydraulic conductivity
Meteorological data		Time lapse GPR	Leakage coefficient
Lateral flow networks verification using discharge data			
Rainfall	ERT: depth to bedrock	Stream discharge	Macropore domain: non-linearity and reservoir constant
Isotopic signature of rainfall	Calibrated EFU parameters	Isotopic signature in stream	Darcy–Weisbach: roughness, pipe diameter, number of parallel pipe networks
Meteorological data			Diffusion wave: hydraulic conductivity
			Hydraulic conductivity of slow groundwater reservoir

units does exist and whether their thorough exemplary experimental structural and functional characterization is helpful to partly reduce inherent equifinality. The ongoing hierarchical verification approach spans from the EFU scale across hillslope and headwater scales (Table 3). In addition to the traditional split sampling tests (calibration/validation periods), the verification approach therefore also comprises parameter transfer tests among EFUs of the same class and hillslopes of the same LTU class. As this verification is a multidisciplinary task, we also put a focus on the identification and development of universally applicable verification criteria and metrics. The major challenge here is to find ways for joint evaluation across variables and scales and to complete established metrics tailored for specific observables.

5.2 Closing word on the value of sharing our failures

The outlined experimental design covers a sufficient number of members of each candidate EFU and LTU class to enable characterization of structural and functional similarities and differences. In combination with the ongoing model verification this constitutes, in our opinion, a strong test for the presented propositions and ideas. We have interesting findings to be published in the forthcoming research papers – some match our expectations, some are truly surprising – which will tell how much of our hypotheses and ideas will be corroborated, will need refinement, or even will be rejected. We take this risk of “being proved wrong” to vote for a publication culture that allows sharing of scientific failures instead of hiding them, simply because there is much to be learned from scientific falsifications. Opinion papers may serve exactly this purpose, among others.

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