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Discussions

HESS Opinions: Functional units: a novel framework to explore the link between spatial organization and hydrological functioning of intermediate scale catchments

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Abstract

This opinion paper proposes a novel framework for exploring how spatial organization alongside with spatial heterogeneity controls functioning of intermediate scale catchments of organized complexity. Key idea is that spatial organization in landscapes implies that functioning of intermediate scale catchments is controlled by a hierarchy of functional units: hillslope scale lead topologies and embedded elementary functional units (EFUs). We argue that similar soils and vegetation communities and thus also soil structures "co-developed" within EFUs in an adaptive, self-organizing manner as they have been exposed to similar flows of energy, water and nutrients from the past to the present. Class members of the same EFU (class) are thus deemed to belong to the same ensemble with respect to controls of the energy balance and related vertical flows of capillary bounded soil water and heat. Class members of superordinate lead topologies are characterized by the same spatially organized arrangement of EFUs along the gradient driving lateral flows of free water as well as a similar surface and bedrock topography. We hence postulate that they belong to the same ensemble with respect to controls on rainfall runoff transformation and related vertical and lateral fluxes of free water. We expect class members of these functional units to have a distinct way how their architecture controls the interplay of state dynamics and integral flows, which is typical for all members of one class but dissimilar among the classes. This implies that we might infer on the typical dynamic behavior of the most important classes of EFU and lead topologies in a catchment, by thoroughly characterizing a few members of each class. A major asset of the proposed framework, which steps beyond the concept of hydrological response units, is that it can be tested experimentally. In this respect, we reflect on suitable strategies based on stratified observations drawing from process hydrology, soil physics, geophysics, ecology and remote sensing which are currently conducted in replicates of candidate functional units in the Attert basin (Luxembourg), to search for typical and similar functional and structural characteristics. A second asset of this framework is that it blueprints a way towards a structurally more adequate

model concept for water and energy cycles in intermediate scale catchments, which balances necessary complexity with falsifiability. This is because EFU and lead topologies are deemed to mark a hierarchy of "scale breaks" where simplicity with respect to the energy balance and stream flow generation emerges from spatially organized process-structure interactions. This offers the opportunity for simplified descriptions of these processes that are nevertheless physically and thermodynamically consistent. In this respect we reflect on a candidate model structure that (a) may accommodate distributed observations of states and especially terrestrial controls on driving gradients to constrain the space of feasible model structures and (b) allows testing the possible added value of organizing principles to understand the role of spatial organization from an optimality perspective.

1 Organized complexity and the need for a new framework to characterize and model intermediate scale catchments

1.1 Spatial organization: evidence and fingerprints

Catchments having gradually evolved in a multitude of contrasted environments and climates throughout the world can be seen as evidence of spatial organization being triggered by landscape evolution (Sivapalan et al., 2003a; Phillips, 2006). Catchments delimit stationary areas of "confluence" where driving gradients force vertical and lateral flows of non-bounded "blue water" via a connected river network to the catchment outlet. The integral response behavior of a large control volume can thus be characterized by long term monitoring of mass input (rainfall) and output (river discharge) through a rather well defined cross section. This is a unique advantage of hydrology compared to for instance meteorology, as conceptual rainfall runoff models may focus on solving the water balance, (partly) the land surface energy balance, but treat the momentum balance in a lumped manner. As this parsimonious paradigm allows successful predictions of stream flow response at larger scales, it is fully justified.

A catchment's internal spatial organization manifests through different fingerprints and affects different processes and catchment functions; for instance as deterministic pattern of soil types at the hillslope scale (Milne, 1936; Bushnell, 1942), or a local scale spatial covariance of soil hydraulic properties in a given soil type (Zimmermann et al., 2008). This form of spatial organization in "textural storage elements" translates into spatially correlated storage, partly temporarily stable patterns of soil moisture (Western et al., 2004; Brocca et al., 2007; Blume et al., 2009; Zehe et al., 2010), and spatially correlated, deterministic patterns of infiltration (Zehe and Bloeschl, 2004; Zehe et al., 2005). The most striking evidence for spatial organization is, however, the omnipresence of networks of preferential flow paths, which vein soils and unconsolidated rock. Independently from their genesis, whether they are bio-pores or fingerprints of past erosive and thus dissipative processes, they exhibit similar topological characteristics and similar functioning (Fig. 1). Preferential flow paths hence "organize" distribution and export of water and matter from/within hydrological systems either locally as vertical macropores (Beven and Germann, 1982, 2013), at the hillslope scale as 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 at the catchment scale as river networks (Howard, 1990; Kleidon et al., 2013).

As some readers might wonder about our notion of organization we provide a brief explanation. Organized system configurations can be loosely characterized as being far away from the configuration of maximum disorder, which is characterized by a local entropy maximum (Kleidon et al., 2013). Entropy is closely related to information (Shannon, 1948), which can be measured based on the minimum number of necessary questions to fully characterize a system state or to locate a single object in a large number of possible boxes. The maximum entropy configuration is the one where the object is equally likely in each box (uniform probability density), which is equivalent to a system where all states and properties are uniformly distributed and the local thermodynamic equilibrium (LTE) is reached. Persistent spatial gradients in catchment properties reflect thus a spatially organized configuration far from LTE (Kleidon et al., 2012). A spatial covariance in soil properties and related states is associated with a lower entropy as an uncorrelated random pattern with the same variance, because at separating distances smaller than the range/correlation length we need a smaller number of questions to detect how close two observations of states/parameters might be. In line with this an apparent network of preferential flow paths and the river net itself reflect a system configuration far from LTE, because the inlets and outlet(s) of these networks mark a very small fraction in the system boundaries where runoff/free water either leaves the catchment or might enter and leave the subsurface of a hillslope.

1.2 The challenge of organized complexity in intermediate scale catchments

Jim Dooge (1986) was to our knowledge the first hydrologist who realized that spatial organization alongside with stochastic heterogeneity leads to complex hydrological behavior at intermediate scales between 5 and 200 km^2. Dooge (1986) argued that these catchments are systems of organized complexity; being already too large and heterogeneous to be treated in a reductionist deterministic manner, but yet too small for characterizing their behavior using first and second order statistics. The latter is possible at larger scales of organized simplicity, which is according to Dooge *the* reason why lumped conceptual models work well at this scale.

The hydrological functions of intermediate scale catchments (export and storage of free water, land atmosphere energy exchange and related supply of capillary bounded water) are largely determined by the way how partly organized patterns of storage elements i.e. soil and aquifers and networks of preferential flow path interact and react to meteorological forcing regimes (Phillips, 2006; Schulz et al., 2006; Zehe and Sivapalan, 2009). These “structure-process” interactions are, depending on the system state(s), associated with threshold-like changes in catchment functions. This is either due to activation of vertical and lateral preferential flow (Buttle and McDonald, 2002; Tromp-van Meerveld and Weiler, 2008; Wienhöfer et al., 2009; Fujimoto et al., 2011) or mobilization of pre-event water due to pressure transduction (e.g. Bonell et al., 1990; Sklash et al., 1996). Despite the great progress that has been achieved in hydrology of

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hillslopes and at the scale of organized simplicity, we feel that hydrology is still pretty "naked" at the intermediate scale of organized complexity. Mainly because our theoretical picture of how the sketched structure-process interactions control changes in catchment integral response is to date still severely limited by non-exhaustive measurement technology and concepts (Beven, 1996, 2006). Consequently, we struggle to invert on the underlying structure-process interactions when observing signatures of such transitions in catchment integral behavior. This in turn explains the lack of rigorous theoretical concepts to represent threshold changes and emergent behavior in hydrological models.

Closing this gap at the lower mesoscale is more than "just" of academic interest. Hydrological practice often avoids operational flood forecasts in intermediate scale catchments because of the highly uncertain rainfall predictions *and* the deficiencies of rainfall runoff models at this scale. Furthermore, it becomes increasingly important not only to predict the response behaviour of catchments for the status quo, but also to project how changes of the climatic conditions and the hydro-ecosystem system itself will translate into altered hydrological functioning (Sivapalan et al., 2003a; Zehe and Sivapalan, 2009; Tiejten et al., 2010; Ehret et al., 2014). The latter requires stepping beyond input-output models as hydrological system changes are spatially distributed. Last but not least, measures for global change impact mitigation are deemed to be most effective at intermediate scales, as their sizes correspond to the smallest administrative units. This calls for appropriate and specific research and modelling at exactly this scale.

1.3 Rationale and structure of this paper

In this paper we propose that spatial organization in catchments and their evolution implies the existence of functional landscape entities, which pave the way to unify experimental characterization and modeling of complex catchment behavior at intermediate scales. Why so? Formation of the above specified organized patterns and networks of preferential flow paths in a distinct geological setting has been strongly affected by past water and energy flows (Phillips, 2006; Savenije, 2010) as well as by the co-evolution of distinct natural communities (Watt et al., 1947; Schröder, 2006; Schaefli et al., 2010; Troch and Harman, 2013). Does similarity of organized patterns and preferential flow networks thus imply that past process patterns have been similar in the sense of the pattern-process paradigm from theoretical landscape ecology (Watt et al., 1947; Schröder, 2006)? If so, it seems logical that structurally similar landscape entities at different scales (pedons, hillslopes, headwaters) exert also at present similar controls on distributed dynamics. This implies that a set of typical dominant flow paths and flow processes could be attributed to structurally similar landscape entities (Winter, 2001; Naef et al., 2002; Gao et al., 2013) and that they would function similarly when they have been exposed to similar forcing conditions.

The idea about functional landscape entities, often named **h**ydrological **r**esponse **u**nits (Flügel 1996), is not new and a large set of HRU separation methods have been suggested. Although HRU identification has nowadays merely degenerated to a GIS-clipping exercise, we regard the core idea nevertheless as very appealing as it points a path to link stratified observations, landscape structure and model concepts. Our new concept is in line but goes also clearly beyond the original idea of HRUs, which neglects for instance their lateral exchange driven by superordinate gradients as criticized by Neumann et al. (2010). We postulate that a hierarchy of functional units, lead topologies and elementary functional units (EFU), compile the main catchment functions in a given hydrogeological setting by spatially organized interactions at and across different scales. We propose that these functionally similar units are characterized by similar soils and vegetation communities which have co-developed in an adaptive manner along a hierarchy of similar gradients that have caused similar energy and water flows from the past to the present. We thus expect members of the same EFU class to belong to the same ensemble with respect to the first order controls of land atmosphere energy exchange and the supplying vertical fluxes of capillary soil water and heat. EFUs are embedded in superordinate lead topologies, whose class members are deemed to function similarly with respect to hillslope scale rainfall runoff generation and the sustaining vertical and lateral flow processes of free water (compare Sect. 3.2). We expect class members of EFU and lead topologies to have a distinct way how their architecture controls the interplay of state dynamics and integral flows, which is typical for all members of one class but dissimilar among the classes. This implies that we might infer on the typical dynamic behavior of the most important classes of EFU and lead topologies in a catchment, by thoroughly characterizing a few members of each class.

We expect EFU and lead topologies, assuming that they exist, to be key elements/objects of a structurally more adequate model concept for water and energy cycles in intermediate scale catchments. We believe them to mark a hierarchy of "scale breaks", where simplicity with respect to the energy balance and stream flow generation emerges from spatially organized process-structure interactions. This in turn bears the potential for simplified descriptions of these processes which are nevertheless physically and thermodynamic consistent. The proposed framework is currently tested in the Attert basin in Luxembourg within the DFG-FNR Research Unit "**C**atchments **a**s **o**rganised **s**ystems CAOS" (www.caos-project.de). The Attert research basin has been operated in since 1994 by the CRP-Gabriel Lippmann in the framework of its water resources research programmes (e.g. Pfister et al., 2009, 2010; Martínez-Carreras et al., 2012). Beside an excellent hydro-meteorological data set it offers a quite unique range of physiogeographical settings. Here, we intend to discuss the main challenges related to the quest for a hierarchy of functional entities and introduce our initial experimental design. We also propose a candidate model structure based on EFU and lead topologies that (a) may accommodate distributed observations of states and especially driving gradients to constrain the space of feasible model structures and (b) allows testing the possible added value of organizing principles to understand the role of spatial organization from an optimality perspective.

Our initial ideas may be compared with our future findings. With this we cannot "sell" the a-posteriori syntheses of our research as a-priori hypotheses in the follow up papers. This makes scientific learning a transparent none-white-washed process, and

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documents also how much we learn from our failures. In the following we briefly discuss complex functioning at the intermediate scale of organized complexity and related short comings of established paradigms (Sect. 2). Then we explain the main ideas underlying our holistic approach as well as the main elements of our functional classification scheme (Sect. 3) and reflect on implications for modeling and characterization of intermediate scale catchments. The paper closes with an outlook on the ongoing test of the framework in Sect. 4.

2 Specific challenges at intermediate scales

2.1 Spatial organisation and complex functioning

2.1.1 Hillslope scale rainfall runoff generation, preferential flow and non-Gaussian behavior

Hillslopes are key elements that organize stream flow generation in many intermediate scale catchments as their relief controls the potential energy gradients driving downslope flows of free water (In the following we refer to this "water source" as blue water supply, although the term blue water is used in a more strict sense in the virtual water community). Hillslopes are often characterized by a typical topography and a typical soil catena (Milne, 1936; Bushnell, 1942), which determine the spatial pattern of capillary soil water that is stored against and potentially feeds evapo-transpiration. (In the remainder we will loosely refer to this water source as green water supply, although the term is used in a more strict sense in the virtual water community). Networks of preferential flow paths (rills, pipes macropores) facilitate hillslope scale recharge of green and export of blue water by reducing the "control volume flow resistance" towards the driving gradient. This is due to a spatially organized arrangement of soil material assuring connectedness of the flow paths and is not reflected in a change of soil texture and the flow resistance in the soil matrix.

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In intermediate scale catchments time scales of hillslope scale preferential flow and of downstream transport in the river system are of similar magnitude (Wienhöfer et al., 2009; Garcia and Weiler, 2010). Transport distances are thus too small to treat flow and transport in the hillslope subsurface as being well mixed as the central limit theorem does not yet apply. Neglecting the effect of preferential flow at this scale is, thus, as error prone as neglecting the river network itself. As residence time distributions of water and solutes in the subsurface are non-Gaussian (Bloeschl and Zehe, 2005; Neuweiler and Vogel, 2007), the success of predictions depends essentially on an accurate representation of the topology and hydraulic characteristics of subsurface preferential flow paths and of the bedrock in the model structure (Tani, 1997; Fujimoto et al., 2011; Klaus and Zehe, 2011; Wienhöfer and Zehe, 2014). This is in principle possible with reductionist physically based models. However, the required information is not directly observable (compare Sect. 2.2) and to a certain extent unique for each place (Beven, 2000). Most networks of preferential flow paths are created by biota such as earthworms (Lavelle et al., 2006; Meysman et al., 2006), ants and plant roots. A key towards estimating their density and topology at the catchment scale might be to understand the habitat factors and their interactions, which determine behavior, population dynamics and dispersal of key ecosystem engineers such as earthworms, ants or rodents (Jones et al., 1994; Hastings et al., 2007; Schröder, 2008).

Conceptual models, at least those which treat the subsurface as a series of well mixed reservoirs, are structurally inadequate to deal with preferential flow at intermediate scales.

2.1.2 The momentum balance and mobilization of pre-event water

Displacement of "old" pre-event water is an emergent phenomenon that may significantly control runoff production and associated transport of nutrients and contaminants at hillslopes and in intermediate scale catchments (Sklash and Farvolden, 1979; Cloke et al., 2006; Wenninger et al., 2004; Blume et al., 2008; Graeff et al., 2009; Klaus et al., 2013). The "old/new water paradox" (Kirchner, 2003) is, however, no paradox in

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the light of the momentum balance. Mobilization of pre-event water by means of pressure transduction is controlled by the specific storage coefficient of the aquifer (Tetzlaff et al., 2012), which is as a hydraulic property linked to the subsurface momentum balance. The speed of compression waves is several orders of magnitude larger than subsurface particle flow velocity. It is therefore no paradox that old water close to the stream-aquifer-interface can be quickly "pushed" into the stream by pressure waves.

Many conceptual rainfall–runoff models focus on solving the water balance, (partly) the land surface energy balance, but represent the momentum balance by lumping "driving gradients" and "flow resistances" into reservoir constants. This paradigm allows successful predictions of stream flow response at the scale of organized simplicity, because the catchments concentrate blue water flows in the above specified manner to the outlet. Neglecting explicit treatment of the momentum balance has, however, not only the "academic" drawback to be confined in the old new-water paradox. Also the problem of equifinality (Beven and Binley, 1992) can partly be attributed to a lumped treatment of "driving gradients" and "flow resistances", as explained in Sect. 2.2.1.

2.1.3 Land–atmosphere energy exchange, evapo-transpiration and green water supply

Evapo-transpiration is the only process that can drain the soil beyond field capacity/soil hydraulic equilibrium. It is as slow mass flux mainly fed by green water. Green water supply depends on soil water retention properties and thus capillary forces on soil water in the "middle fraction" of the pore space, root depth and depth to groundwater. However, evapo-transpiration is, though being a slow mass flux, as latent heat flux "fast" and dominates the land surface energy balance (EBC). In fact evapo-transpiration is driven by the divergence in radiative energy fluxes at the surface, which builds up near surface gradients in air temperature and humidity. Land surface–atmosphere energy exchange is thus rather a feedback than a "sink" were green water is simply lost to the atmosphere.

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A key challenge for hydrological modeling (not only at the intermediate scale) is to better understand what is limiting/facilitating partitioning of net radiation into sensible and latent heat and finally transpiration. Atmospheric turbulence, which depletes humidity and temperature gradients by fast mixing as well as green water supply are the key physical limiting factors. Some key assumptions underlying shallow turbulence parameterization based on Monin–Obukhov-similarity such as horizontal homogeneity and constant turbulent fluxes near the ground are, however, questionable in intermediate scale catchments, especially in case of a pronounced topography. Vegetation can be seen as "preferential flow path" for green water into the atmosphere, as plant roots may extract soil water against steep gradients in soil water potential and thus shortcut dry topsoil layers, which considerably block bare soil evaporation. The functioning and limitation of this biotic "preferential flow path" is however controlled by plant physiology i.e. root water uptake, plant water transport, stomata conductance and gas exchange. Does thus the plant metabolism limit photosynthesis and plant gas exchange (Schymanski, 2009), or is it turbulent transport of CO_2 into the canopy as recently suggested by Kleidon and Renner (2013)? The strong dependence of the EBC on vegetation properties became recently a focus in land system research, because it has been demonstrated that current soil-vegetation models have severe problems in a correct simulation of the EBC (Gayler et al., 2013, 2014; Wöhling et al., 2013; Greve et al., 2013). Key topics are a dynamic simulation of root water uptake and plant growth. Coupling of hydrological models and meteorological models to treat evapo-transpiration as a feedback instead of a sink, is thus more than "just" a numerical problem, it is a theoretical challenge with respect to plant physiology, micro-meteorology and thermodynamics.

2.2 Shortcomings of model paradigms at intermediate scales

Predicting catchment behavior correctly and "for the right reasons" (Seibert and McDonnell, 2002; Kirchner, 2006) means that the model simulates the underlying process structure interactions in a simplified but realistic manner and allows rejecting of hypotheses on how these process structure interactions translate into catchment

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functions. At intermediate scales conceptual models fail in being realistic and reductionist models fail in being falsifiable, as will be explained in the next two subsections.

2.2.1 Conceptual models: getting right answers for unrealistic reasons

The charm of conceptual hydrological models is that they are simple and nevertheless work well. This is because catchment scale rainfall runoff response appears in many places simple and dominated by a few controls, regardless of the rich complexity at the pedon and hillslope scales (Sivapalan, 2003). The main strength of conceptual models is however also their main weakness. As most of them do not disentangle gradients and flow resistances controlling hillslope lateral water flows, they cannot draw advantage from field observations characterizing landscape controls on these gradients. This "physical bias" is reflected in equifinality as sketched in Fig. 2: an increase in bedrock topography can for instance be compensated by decreasing subsurface transmissivity/hydraulic conductivity (i.e. increasing flow resistance) to maintain the same subsurface water flux.

Many conceptual models predict the effect without proper accounting for the cause: a successful reproduction of discharge at the catchment outlet does often not imply that distributed dynamics inside the catchment is simulated in accordance with observations (e.g. Graeff et al., 2012) or in a consistent manner among different acceptable model structures (Tapah, 2009). Even those model parameters which appear observable at first sight – as the root depth in forested areas – cannot a priori be parameterized according to observations or expert knowledge, because the model structure forces them outside physically meaningful ranges. Distributed state observations, process and system understanding are thus not very helpful for constraining conceptual model parameters: modelers and field hydrologists are "lost in translation" (Beven, 2009). At the end of the day we get what we pay for: one cannot expect input output models that were designed to function without measurement details about the catchment structure to take advantage from available information about such details and to move beyond the input-output paradigm. Consequently, they can neither be used to

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predict distributed water driven transport of solutes and erosion (at least not for the right reasons) nor be coupled to atmospheric models to tackle the problem of landsurface–atmosphere feedbacks.

2.2.2 Reductionist model: data greed and lack of falsifiability

Distributed reductionist models commonly describe soil water flow using the Darcy–Richards approach, solute transport using the convection dispersion approach and overland flow/river flow by 1-D or 2-D hydraulic approaches. In principle they allow consistent predictions of internal dynamics and integral flows including non-Gaussian transport based on different conceptualizations of preferential flow up to the headwater scale (Gassman et al., 2013). Taking real advantage from application of these models requires detailed data on soil hydraulic functions, their spatial correlation lengths, the topology of preferential flow paths and related flow resistances, plant morphology and physiology, bedrock topography and much more. The absence of such detailed data, which is unfortunately rather the rule than the exception at intermediate scales, reduces the added value of applying reductionist models considerably. Inverse modeling/calibration as done for Hydro-Geo-Sphere (Perez et al., 2011), Mike She (Christiaens and Feyen, 2001, 2002), or CATFLOW (Klaus and Zehe, 2010) leads (non-surprisingly) to the same problems as for conceptual models. One obtains either effective parameter sets for soil hydraulic functions that strongly differ from those derived within multistep outflow experiments, because these parameters jointly represent matrix and preferential flow (Troch et al., 1993; Hopp and McDonnell, 2011). At the end of the day we are thrown back to calibration and non-commensurable parameters; measured lab data are useless. Or, in case one decides to disentangle matrix and preferential flow there is a strong equifinality in acceptable model structures, also because a large set of different network topologies produce similar response behavior (Binley and Beven, 2003; Klaus and Zehe, 2010; Wienhöfer and Zehe, 2014).

However, even if sufficiently resolved information were available, application of physically based models at scales of intermediate complexity remains a numerical challenge with respect to convergence, stability and accuracy of the numerical approximation. Quantification of predictive uncertainty is rather difficult to achieve due to the large computational costs (Klaus and Zehe, 2010; Reusser et al., 2011; Reusser and Zehe, 2011; Gassman et al., 2013). Falsification of reductionist models appears virtually impossible as the different error sources i.e. equations, parameter fields, numerical solvers, fields of boundary conditions can hardly be understood by a single scientist.

3 A holistic and hierarchical framework to tackle organized complexity

3.1 Our way forward: linking experiment to theory as well as the "how" to the "why"

To close the gap at the lower mesoscale we propose a holistic framework that combines the advantages from both modeling schools (Savenije, 2009) with novel experimental strategies to explore how spatial organization alongside with spatial heterogeneity controls functioning of intermediate scale catchments. "Holistic" means for us to link the "how" to the "why" by drawing from generic understanding of landscape formation and biotic controls on processes and structures as well as to rely on exemplary experimental learning in a hypothesis and theory based manner. Our framework builds on three main hypotheses H1 to H3.

H1: Spatial organization in landscapes implies that functioning of intermediate scale catchments in a given geological setting is controlled by a hierarchy of functional units: hillslope scale lead topologies and embedded elementary functional units (EFUs). We expect that similar soils and vegetation communities and thus also soil structures "co-developed" within EFUs in an adaptive, self-organizing manner as up to the present they have been exposed to similar flows of energy, water and nutrients. Class members of the same EFU (class) belong to the same ensemble with respect to the controls of the energy balance and related vertical flows of green water and heat (Table 1). Class members of superordinate lead topologies

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exhibit the same spatially organized arrangement of EFUs, and a similar surface and bedrock topography. They hence belong to the same ensemble with respect to the controls on rainfall runoff and related vertical and lateral fluxes of blue water. Functional similarity implies that the typical dynamic behavior of the most important classes of EFU and lead topologies in a catchment might be understood, by thoroughly characterizing a few members of each class.

H2: A joint treatment of mass, energy and the momentum balance is the key to break out from the input-output paradigm and to include stratified observations, conducted to detect and characterize functional units, into the model identification process. The EFU and hillslopes scale is the key to formulate processes descriptions for the energy balance and rainfall runoff which balance complexity and falsifiability. This is because the internal organisation of EFU's and lead topologies, due to an apparent spatial covariance and preferential flow paths, translate into local homogeneity, as well as anisotropy and a dominating direction of green and blue water flows. This would imply a reduced dimensionality of the problem, partly a simplified coupling of vertical and lateral flow across scales. The related model object structure and reduction in process complexity is a falsifiable hypothesis.

H3: Organizing principles such as maximum entropy production or maximum power (Lotka, 1922; Paltridge, 1979) are a key to link the "how" to the "why" question. Testing the explanatory and predictive power of such principles requires thermodynamic consistency, i.e. that any flux is equal to a potential gradient divided by resistance, and explicit treatment of flow in preferential flow paths. This assures that the model may track (free) energy conversions and dissipation associated with mass fluxes sustaining blue and green water dynamics and related preferential flow processes.

In the following section we will explain the main thoughts underlying these hypotheses and discuss their implications for characterization and modeling of intermediate scale catchments.

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3.2 Catchment functions and their corresponding functional units

We distinguish three main integral catchment functions: (1) blue water storage and release by base flow, (2) land–atmosphere energy exchange and related green water supply and heat fluxes, as well as (3) runoff generation, related blue water flows and green water recharge during rainfall events. H1 postulates that a hierarchy of different functional units controls these different catchment functions. Their operative control does however change with the prevailing forcing (Fig. 3). This is because these integral functions operate in different prevailing contexts (radiation/rainfall driven), and differ with respect to the strength, nature and direction of the driving gradients (Table 1) and with respect to the characteristic spatial and temporal scales of the dominant processes and the type of dominant structures.

Control volumes are defined as functionally similar and thus belonging to a functional unit, if they share the same dominant flow processes and respond with similar flow of mass and/or energy when being exposed to a similar forcing. Plant communities that consist of similar functional groups and are in the same age are expected to function similarly with respect to biomass production, exchange of CO_2 and transpiration when being exposed to identical forcing conditions (Lavorel and Garnier, 2002). Soil profiles that evolved under similar conditions from the same parent material are expected to function similarly with respect to upward and downward green water and heat fluxes at least in the soil matrix continuum. Similarity with respect to a distinct function arises from similarity with respect to those structures that control the gradients and resistances determining the dominant processes.

3.2.1 Hierarchy level I: sub-catchment scale blue water storage and base flow organization by hydrogeological and morphological setting

The highest level of our functional classification scheme is the hydro-geological and geomorphic setting of sub-catchments. This determines the starting point for morphological processes and constrains thus the set of hillslope forms (including surface and

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subsurface topography) as well as parent rock for soil formation. It determines furthermore hydraulic characteristics of the aquifer, therewith sub-catchment blue water storage, base flow characteristics, the slow branch of the residence time distribution and thus the nature of the catchment memory. This is nicely illustrated by the annual plots of cumulated discharge against cumulated rainfall that are presented for two sub-catchments of the Attert (Fig. 4), which is located on the border between the schistous Ardennes massif and the sedimentary Paris Basin (Pfister et al., 2002). The Hueweler-bach acts like a low pass filter with very long linear memory, which is controlled by the huge fractured sandstone aquifer. The Weierbach, located in schist, has in contrary a much shorter and non-linear memory in its annual rainfall runoff behavior because flow is controlled by storage in a much thinner layer of weathered schist on top of impermeable bedrock (Fig. 4).

3.2.2 Hierarchy level II: stream flow generation organized within hillslope scale lead topologies

Within a given hydro-geological setting we distinguish hillslope scale lead topology classes (Fig. 4b). Class members are deemed to belong to the same ensemble with respect to event scale stream flow generation/rainfall runoff generation; i.e. they share the same dominant vertical and lateral blue water flow processes and can be characterized by a similar resident time distribution. As blue water flows are driven by differences in potential energy, hillslopes are the key organizing element for this function. Their surface and bedrock topography and morphology alongside with soil and bedrock permeability determine whether/how fast a free surface or subsurface water table builds up and if so, the steepness of the water level gradient driving lateral flow. As suggested by Zehe et al. (2013), rainfall runoff transformation is facilitated by preferential flow in drainage networks which act like veins. These are preferential flow networks that connect the soil surface (blue water source areas) in the slope directly to the riparian zone. On the other hand we have dead ended macropores such as roots and earthworm

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burrows which facilitate green water recharge as they redistribute water within the soil matrix acting like arteries.

Candidates for lead topology classes consist thus of similar hillslopes (with respect to surface and subsurface topography and morphology, land use) *that are* interconnected to similar riparian zones (Fig. 3b; located at similar at a similar reach of the stream network) This implies that up to now similar conditions have affected sediment redistribution and formation of the soil catena, (possibly) surface rill networks and formation of the riparian zone. We expect also similar conditions to have affected internal erosion and the formation of lateral pipe networks. The search for candidate lead topologies is difficult, as neither lateral and vertical preferential flow paths nor the topography and permeability of the bedrock interface are directly observable. But this case is also not hopeless as explained in Sect. 3.3.1.

3.2.3 Hierarchy level III: land surface energy balance organized by elementary functional units (EFU)

We furthermore propose that several elementary functional units EFU are arranged along these lead topologies in a spatially organized manner (Fig. 4c). Members of a distinct EFU class are deemed to belong to the same ensemble with respect to the land surface energy balance and the related vertical fluxes of (green and blue) water and heat. The main driver for the land-surface energy balance is the net radiation (i.e. divergence of radiative fluxes). Candidate class members are characterized by a plant and soil albedo, which is expected in case of a similar vegetation community, as well as similarity in global radiation input determined by aspect and slope. Partitioning of net radiation into latent and sensible heat depends mainly on the functional vegetation community and the green water supply. Green water supply and vertical green water fluxes are controlled by gradients in soil water potentials, especially gradients in capillary binding energy/matric potential. This in turn depends on the soil water retention curve(s) and soil hydraulic conductivity curve(s) of the apparent soil profile, the soil moisture profile and depth to groundwater.

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We propose that in pristine areas different EFU classes have developed along a given hillslope due to a self-organizing adaptation of plant communities and hydro pedological characteristics (Troch et al., 2013; Harman and Troch, 2013). 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 (past water, energy and nutrient flows) causing formation of typical soil profiles with distinct soil texture and matrix properties in different horizons. This implies, depending on hillslope position and aspect, formation of distinct niches with respect to water, nutrient and sun light availability and thus “filters” to select distinct natural communities of plant and small animal species (Keddy, 1992; Poff, 1997; Schröder, 2006). 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 vertical and lateral flows of water, mass and thermal energy. Searching for EFUs in pristine areas requires thus identification of plant communities, representative soil textural properties of the main catena elements and abundance of ecosystem engineers creating biotic macropores. In non-pristine landscapes either agricultural practice or forest management might play a dominant role for detecting EFUs. This human influence determines an additional disturbance regime for wild plants and animal species, and controls either the age spectrum and species composition of tree species in forest areas or surface preparation, optionally cutoff of macropores and selection of crops in agricultural areas.

3.3 Experimental challenges and implications for characterization of functional units

The concept EFUs and lead topologies can be seen as a generalization of the HRU idea which steps beyond its limitation of neglecting lateral exchange. We provide furthermore a clear definition of functional similarity, how this relates to bio-physical similarity of the landscape, the nature of the forcing and the driving gradient. The biggest advantage of our concept is, however, that it is an experimentally testable hypothesis

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(compare Sect. 4.1). When testing the concept of functional units, we face the same problems that the community has been struggling with since the HRU concept has been proposed by Flügel (1996). Up to now, a large set of HRU separation methods has been suggested as for instance topographic indicators to support geomorphology based predictive mapping of soil thickness (Pelletier and Rasmussen, 2007), 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, landuse and small-scale experiments for agricultural land (Naef et al., 2002; Schmocker-Fackel et al., 2007). However, an experimental test of the HRU concept is to our knowledge still missing.

3.3.1 Balancing extent and support of the observation network and link similarity across scales

One key challenge to test H1 is to balance the need for exhaustive characterization of structure process interaction within EFU class members with the need to conduct replicate experiments or monitoring to detect typical functional and structural characteristics. Members of a candidate EFU class must show a similar interplay of the energy balance and related green water dynamics, while different classes behave distinctly dissimilar. For instance means and variances of sap flow, soil moisture and soil heat dynamics should be identical within the confidence limits when class members have been exposed to a similar meteorological forcing. Members of the same lead topology class should produce a similar stream flow contribution while different classes behave distinctly dissimilar. We thus expect that class members share the same dominant flow processes and residence time/travel time distributions when they have been exposed to the same meteorological forcing for a time sufficient to assure a similar state.

To test H1 we propose stratified multiple observations from process hydrology, soil physics, geophysics, ecology and remote sensing in a design that cuts across scales without cutting off the flow paths (compare Sect. 4.1). Hillslopes are perfect focus areas to cluster such stratified multiple observations as they are clearly separable with respect to their catena, ecological and geomorphic properties and consist of several EFUs. Hillslopes large enough to identify typical macroscopic patterns of key properties controlling rainfall and radiation interception, green water supply to transpiration and blue water supply to stream flow generation. On the other hand, they are still small enough to conduct identical experiments and monitoring within different replica of the same candidate lead topology to identify typical structural and functional characteristics.

The second challenge when testing H1 to explore how spatial organization in landscapes controls rainfall runoff transformation in intermediate scale catchments is that we need to link similarity across four orders of spatial extent (from EFUs to catchments). As a matter of fact, the majority of tracer-based investigations on runoff processes have been carried out to date in small ($< 10\,km^2$), 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, 2010) and headwaters to meso-scale ($\sim 200\,km^2$) catchments. McGuire et al. (2005) 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. Viville et al. (2006) reported for the Vosges Mountains in France a strong control of geology (i.e. fractured bedrock thickness) on MTT. For a set of 20 headwater catchments ranging from < 1 to $35\,km^2$, Hrachowitz et al. (2009) have found strong climate (precipitation intensity) and landscape (soil cover, drainage density, topographic wetness index) controls on MTT.

3.3.2 Geological controls on catchment storage, mixing and residence time

While geological factors have been omnipresent in MTT scaling studies, only few investigations have been able to identify distinct geological differences across nested- and neighbouring catchments. In this respect, investigations targeting geological control

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on flow have brought new insights. Grant and Tague (2004) were able to show in the 30 000 km^2 Willamette basin (Oregon, USA) how the percentage of given rock types in sub-catchments largely controlled the variance of summer low flow. Along the same lines, Sayama et al. (2011) demonstrated in their 17 nested catchment set-ups (3 to 111.7 km^2 in Northern California) how geology and topography control dynamic catchment storage (determined via a catchment water balance).

Bedrock geology has been identified as exerting considerable control on mean residence time. However, the range of bedrock geologies, streamflow and isotopic tracer data covered by the vast majority of past investigations was too small for drawing quantitative conclusions related to geological controls on water storage, mixing and release by catchments. In this context, we ask the question of how catchment physiogeography – and more precisely geology – affects catchment water storage, mixing and release across scales. In the framework of our research project, we build upon insights gained from previous studies in the nested catchment set-up of the Attert basin. We can rely on 9 catchments (sizes ranging from 0.47 to 249.61 km^2) that have combinations of clean- and mixed geologies ranging from schists to marls, sandstone and limestone. Eventually, we expect to infer from information related to storage, release and isotopic signatures (in precipitation and stream flow) in our nested catchment set-up to gain new understanding on what controls dominate storage, mixing and release differences across catchments and scales.

3.3.3 Lead topology identification and characterization

Key determinants for members of candidate lead topologies are, beside similar surface attributes (catena, topography, vegetation, land use), also a functionally similar network of lateral and vertical drainage structures as well as a similar topography and permeability of the bedrock interface. Although these signatures are not directly observable, we may combine geophysical proxies (ground penetrating radar, electric resistivity tomography, seismic sounding) with augers to estimate bedrock topography. We may furthermore detect fingerprints of preferential flow in drainage structures for instance

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in the higher moments travel time distributions (McGuire and McDonnell, 2006) from artificial tracer tests or stable isotope data. A way towards using such information for constraining the hillslope scale architecture in our models is to use these models in a forward mode as learning tools to explore how differences in bedrock topography and permeability together with different topologies of preferential flow paths affect different parts of residence time distributions (Wienhöfer and Zehe, 2014). Based on such insights one could infer on the set of hillslope subsurface architectures that could cause a distinct observed signal.

The main challenge when characterizing rainfall runoff behavior of lead topologies is to detect when, how and why hillslopes contribute to stream flow generation. Hillslopes might, for example, be connected directly to the stream network under very dry conditions that turn the soil surface hydrophobic and thus causing overland flow or during very wet conditions leading to high groundwater tables and thus causing subsurface connectivity, while in-between such states the hillslope may be disconnected (Jencso et al., 2010; Bachmair et al., 2012; Tromp van Meerveld et al., 2006; Graham et al., 2010). In recent years promising new investigation techniques have been proposed to complete this puzzle: DTS surveys of groundwater inflow locations along streams (Selker et al., 2006; Westhoff et al., 2007), thermal IR imagery of saturated area dynamics (Pfister et al., 2010; Schuetz and Weiler, 2011), detection of surface runoff onset and cessation in the hillslope, riparian zone, stream continuum with biological tracers (Pfister et al., 2009), geophysical approaches (Graeff et al., 2009), radon as a tracer of groundwater input and extensive observation networks (e.g. Jencso et al., 2010; Tromp van Meerveld et al., 2006).

3.3.4 EFU identification and characterization

Important landscape characteristics to identify members of candidate EFUs are similarity of the “mother” lead topology, hillslope position, functional vegetation (its albedo and plant physiological properties), as well as of the hydropedological characteristics of typical soil profiles (typical retention curve(s) and hydraulic conductivity curve(s)).

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We suggest that green water recharge is mainly facilitated by wetting structures/dead ended macropores (Zehe et al., 2013), for instance earthworm burrows or the plant roots itself, which funnel stem flow in a distributed manner into the root zone. Although, drainage structures facilitate blue water export during rainfall driven conditions and reduce green water supply by a bypass of the soil matrix they are deemed to be of minor importance for green water fluxes sustaining the energy balance during radiation driven conditions.

The search for representative soil textural properties is hampered by the spatial heterogeneity of the soil. EFU class members can at best belong to the same ensemble with respect to soil matrix properties, which implies ergodic conditions are reached and the EFU is much larger than the covariance length of soil hydraulic parameters and of the spatial pattern of tree vegetation, rooting depth and throughfall. At grassland sites the correlation lengths of hydraulic properties are in the order of a few meters (Zimmermann et al., 2008; Zehe et al., 2010), in forested sites they might be determined from spatial patterns of tree density, soil moisture profils (Graeff et al., 2010) and throughfall to tens of meters (Gerrits et al., 2010). Most helpful to judge similarity with respect to density of wetting structures is data on the abundant functional vegetation and on the key ecosystem engineers that create biotic macropores such as earthworms and rodents (van Schaik et al., 2014).

Distributed soil temperature and moisture observations allow observation of heat and green water fluxes, but also help to understand the lateral extent up to which soil water potentials can be deemed as homogeneous, especially under radiation driven conditions. Field studies of Brocca et al. (2007, 2009), Blume et al. (2009) and Western et al. (1998) report that ranks of distributed soil observations within the probability distribution do not change over time. Zehe et al. (2010) found consistent results for two sites of 20 by 20 m^2 were ranks of the distributed soil moisture time series were stable in time, especially during radiation driven conditions. This persistent soil moisture pattern implies that matric potential must be rather homogeneous at this scale. Otherwise small

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scale soil moisture variability would be depleted by lateral soil water flows driven by lateral matric potential gradients.

3.4 Theoretical challenges and the promise of organizing principles

3.4.1 Balancing model complexity vs. falsifiability

The main theoretical challenge is to balance the necessary model complexity vs. falsifiability. How much complexity needs to be added to conceptual models to remove their physical bias and expand them for reliable predictions beyond the input-output paradigm? A simplified but unbiased accounting for the momentum balance, as recommended in H2, does not necessarily imply to 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 properties control those gradients and resistances determining runoff generation and concentration inside the catchment.

Although such conceptual model structures break out of the input-output paradigm, they are too simple to test the predictive power of thermodynamic organizing principles as recently shown by Westhoff and Zehe (2013). The core idea of H3 is that a better understanding of the "why question" – whether catchments have been shaped according to an organizing principle – is ultimately helpful to better predict "how" process-structure interactions control catchment functions. Testing organizing principles based on thermodynamic optimality requires thermodynamic consistency (Kleidon et al., 2012, 2013), i.e. that any flow is driven by a gradient of an intensive state variable such as pressure head, soil water and plant water potentials or soil temperature (Fig. 2). Organizing principles allow us to optimize model parameters with respect to a related objective function derived from this principle. This might be maximization of power or entropy production in a single or all fluxes (Porada et al., 2011; Westhoff and Zehe, 2013; Westhoff et al., 2013), or maximization of net carbon profit of vegetation (Schymanski et al., 2009). The related optimum model structures might allow acceptable non-calibrated predictions of rainfall partitioning into green water supply or overland flow (Zehe et al., 2013) or, in the second case, the prediction of evapo-transpiration and gas exchange (Schymanski et al., 2009).

Reductionist models are thermodynamically consistent, but how much complexity needs to be removed to improve their falsifiability without introducing a physical bias? Falsifiability can be achieved by stating clear hypotheses on how (a) spatial organization reduces dimensionality of the flow problem, (b) how to account for preferential flow paths in explicit manner and (c) how to couple model components for vertical and lateral flows. This way the related reduction in model complexity becomes a falsifiable hypothesis as explained in Sect. 4.2.

3.4.2 Organizing principles and biotic controls on energy exchange

Organizing principles have much to offer to explain biochemical and physical trade-offs and limitations, and to possibly improve predictions of vegetation controls on the water balance. Eco-hydrology provides numerous pioneering examples addressing the question whether life organizes itself in such a way that its functioning is optimal under given habitat conditions. This hypothesis can be tested by taking into account competition between for instance different plant species or trade-offs between fluxes that are driven by different gradients. This competition should then be translated into an objective function. For example, Rodriguez-Iturbe et al. (1999), Porporato et al. (2001) and Caylor et al. (2009) minimized water stress as the objective function for vegetation in (semi-)arid areas. Maximum transpiration and minimal water and oxygen stress have been used by Brolsma and Bierkens (2007), who simulated the competition between two plant species, while Schymanski et al. (2009) optimized net carbon profit under given environmental conditions. The latter builds on the proposition that living systems maximize their energy throughput in order to maximize their ecological fitness (Lotka, 1922). Non-equilibrium thermodynamics and optimality can even be employed to characterize soil development and the functioning of the critical zone (Rasmussen et al., 2011; Rasmussen, 2011; Lin, 2010a, b; Kleidon et al., 2012).

3.4.3 Organizing principles for preferential flows and rainfall runoff

Preferential flow accelerates flow against the driving gradient and thereby its depletion. Thermodynamic organizing principles such as maximum power or maximum entropy production may thus be very helpful in explaining and predicting preferential flow (Kleidon et al., 2013; Zehe et al., 2013). These principles analyze energy conversions and dissipation associated with the rainfall–runoff process or the radiation balance: namely conversions of radiation energy, potential energy, kinetic energy of water flow in channels and capillary binding energy of soil water (Kleidon et al., 2012). Conversions of potential and capillary energy associated with rainfall runoff formation are two orders of magnitude smaller than those energy conversion associated with energy balance. Nevertheless, they provide a key for better understanding of the different functions of preferential flow in cohesive and non-cohesive soils and allow un-calibrated predictions. Zehe et al. (2010, 2013) provided evidence that spatially organized patterns of soils and macropores observed in real world landscapes are in close accordance with thermodynamic optima, either expressed 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. Kleidon et al. (2013) recently showed that the formation of connected river networks maximizes power in steady state sediment flows. Schlüter et al. (2012) investigated infiltration and fingering using thermodynamics and suggested its use for a better upscaling of preferential flow.

4 How to test the proposed framework?

In summary we propose that a thorough understanding of the behavior of a few representatives of the most important EFU classes, their interactions within lead topologies, as well as of how and when the lead topologies connect to the river, contribute to close the gap in our understanding of how distributed dynamics alongside with spatial organization translate into integral catchment behavior. We suggest that a hierarchical

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combination of the related model objects, which are based on simplified but thermodynamically consistent process descriptions, with a river network and a groundwater domain, results in a structurally more adequate model framework for intermediate scale catchments of organized complexity. This approach benefits strongly from distributed observation to delineate and characterize EFUs and lead topologies. One key advantage of our framework is that it can be tested based on replicates of field experiments, monitoring, and modeling of several members of candidate EFUs and superordinate lead topology classes:

- Members within a candidate EFU class should show a similar interplay of green water dynamics and vertical flows controlling the energy balance, while different classes should behave distinctly dissimilar. More concrete we expect class members to belong to the same ensemble, i.e. means and variances of sap flow, soil moisture and soil heat dynamics should be similar when class members have been exposed to a similar meteorological forcing;

- Members of a lead topology class should have a similar stream flow contribution while different classes behave distinctly dissimilar. We expect class members to belong to the same ensemble, i.e. the dominant flow processes and residence and travel time distributions of blue water on its way to the stream should be similar when they have been exposed to a meteorological forcing;

- The structural and functional model parameters that are necessary to reproduce the underlying structure processes interactions are transferable among members of an EFU class as well as lead topology class.

The cardinal challenges when implementing such a test of concept in a catchment, as it is currently done in the Attert basin in Luxembourg in the framework of the CAOS project, are:

- How to observe controls on gradients, flow resistances and how to observe fluxes within members of candidate EFUs and lead topologies by combining geo- and

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soil physical methods, tracer methods, with geo-ecological survey in a representative manner and how to work out the minimum necessary experimental effort?

- May we relate subsurface characteristics observed with geophysics to surface characteristics detected with remote sensing, which might pave the road to regionalize subsurface characteristics using remote sensing up to the catchment scales?
- Which kind of metrics are suitable to quantify functional similarity of distributed state dynamics and integral flows?
- How to discriminate spatial variability in rainfall and radiative forcing, which will cause dissimilar behavior of class members of functional units and could lead to an error of the second kind (rejecting the right hypothesis)?
- How to establish a link between similarity at the hillslope scales and similar integral behavior of catchments, for instance explored within a nested catchment approach?
- What are the necessary model objects, process domains and which process representations are needed to simulate process- structure interactions sustaining the land surface energy balance at the EFU scale and stream flow production at the lead topology level as complex as necessary but as parsimonious as possible?

In the following, we will briefly describe our first guess experimental approach and first guess structure of the CAOS model framework.

4.1 Experimental design in the Attert Basin

To test our hypotheses we conduct identical experiments and monitoring within different replicates of the same candidate EFU and lead topologies in different geological settings of the Attert basins in Luxembourg. The idea is to search for repetitive structural,

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dynamical and functional characteristics, which is the key to understand whether our descriptors for structural similarity of EFUs and lead topologies suggested in Sect. 4.2 constrain indeed functional similarity depending on forcing and state.

4.1.1 Candidate lead topologies and functional units in the schist area

Cornerstone of the permanent monitoring within each member of the candidate EFU and superordinate lead topology are automated sensor clusters, which are further described in Sect. 4.2.3. Instrumentation started within the Colpach sub catchment, a major tributary of the Attert, which is entirely located on schist. While most of the experimental effort has been focused on the schist area (23 sensor clusters), the sandstone and marl areas were also instrumented with 12 and 11 clusters, respectively. Based on a joint analysis of ecological, land use, pedological data, and geomorphic properties, including those determining rainfall and global radiation interception, we selected candidate lead topologies. For the schist area this includes:

– *Short hillslopes with small riparian zone and deciduous forest with shallow Cambisols.* This lead topology is characteristic for forested head waters of the northern part of the Colpach catchment. We distinguish northern and southern aspect, as different soil structures could have developed in response to the different energy input, biomass production and litter fall. We hypothesize that subsurface storm flow dominates stream flow generation during rainfall events. Bedrock topography of the schist interface is thus deemed to be the most important time invariant determinant for the driving lateral gradient. The thickness of the weathered schist layer on top of the bedrock together with its porosity and lateral permeability determine the maximum storage volume as well as the lateral flow resistance for subsurface storm flow. Basic instrumentation of members of lead topologies requires five sensor clusters, as the north and south facing hillslopes share the same small riparian zone.

– *Confluent hillslopes with small riparian zone and pasture with shallow Cambisols.* This lead topology is characteristic for "the source areas" i.e. the head waters of the southern Colpach catchment and thus characterized by convergent flow paths and temporary wetlands in the near-stream and source areas. Bedrock topography is also likely to be of importance here.

In terms of elementary functional units, which are monitored by sensor clusters in the schist area, this amounts to 6 EFUs on north facing slopes and 10 on south facing slopes, 7 EFUs are situated close to a stream, and we included 16 forest and 7 pasture sites (see Table 2). With this design a sufficient number of members of each class are ensured to enable characterization and differentiation of EFUs.

In total we instrumented four replicates of the first lead topology and two of the second and then characterized their structure and dynamic behavior as explained below.

4.1.2 Structural and ecological characterization of lead topologies and EFUs

We are employing electrical resistivity tomography and ground penetrating radar surveys for a rapid assessment of subsurface structures and properties (Fig. 5). These geophysical surveys allow for imaging subsurface architecture along selected 2-D profiles or within selected 3-D subsurface volumes at our field sites. This is to test whether depth to bedrock is indeed similar within the members of the first-guess lead topologies and whether the weathered schist layer exhibits a similar thickness. Furthermore, we derive a distributed functional soil map; i.e. the soil water retention and unsaturated hydraulic conductivity curves for the hydro-pedological units based on soil profiles, augers, undisturbed soil cores and available pedo-transfer functions. Again, we will test whether we find typical curves for the EFU classes.

We shed light on the role of preferential flow paths by means of staining of flow paths using brilliant blue as dye tracer. This is combined with an ecological survey of the abundance and number of individuals of soil ecosystem engineers creating vertical and lateral preferential flow paths, i.e. different earthworm species as well as small rodents, in a randomly stratified design considering the gradients of different habitat factors (Schröder, 2008). This data will serve as a basis for models predicting the spatiotemporal distribution of these species (Palm et al., 2013). The species distributions are then related to distribution patterns of biogenic macropores (van Schaik et al., 2014) and subsequently to hydrological model parameters, using information from infiltration patterns (van Schaik, 2009). The resulting models allow for a comparison of ecological conditions between different EFUs and lead topologies and an improved understanding of interactions between species distributions and soil hydrology.

4.1.3 Monitoring of distributed dynamics and stream flow generation within EFUs and lead topologies

The sensor clusters (Fig. 6) allow observations of a variety of different fluxes and state variables above and below ground one to five tipping bucket rain gauges (Davis Instruments, Rain Collector II); climate sensors for air temperature and relative humidity (Campbell CS215), wind speed (Gi II WindSonic Ultrasonic Wind Sensor), global radiation (Apogee Pyranometer SP110); ten sensors measuring soil moisture (Decagon 5TE), electric conductivity (EC) and soil temperature in depth profiles (Decagon MPS-2); three matric potential sensors (Decagon Devices MPS-2) next to the soil moisture sensors; four water level sensors incl. temperature and EC to observe groundwater and stream water level fluctuations (Decagon CTD); five sap flow sensors to estimate transpiration fluxes (East 30 Sensors). The sensor clusters thus provide temporarily resolved information on fluxes (rainfall/through fall, global radiation, radiation balance, sap flow) and on EFU scale mean and variability of state variables, controlling potential gradients and subsurface flow resistance (temperature, soil moisture, matric potentials, water levels).

Stream flow contribution from candidate lead topologies is characterized by means of stable isotopes, including distributed sampling within soil profiles covering the soil catena, artificial tracer tests, the use of diatoms as smart tracers and radon data. This is combined with repeated incremental discharge observations along the stream during

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average, high and low flow periods, to shed light on exchange processes between lead topologies/hillslopes and the stream. Synthesizing these data with distributed observations of piezometric heads and soil moisture during rainfall events will tell whether the interplay of distributed storage dynamics and event-scale stream flow generation within the same lead topology class is indeed similar and distinctly dissimilar from the behavior of other classes. Crucial for this similarity assessment is to detect the spatial variability of meteorological conditions, which may cause dissimilar behavior even if the concept is feasible (compare next section) as well as identification of proper similarity metrics.

4.1.4 Characterizing energy balance components, phenological controls as well as rainfall variability from EFU to the catchment scales

During radiation-driven conditions horizontally averaged sensible and latent heat fluxes are observed by means of a scintillometer. This will be combined with observations of (a) an energy balance closure station to be installed in the Attert basin, (b) sap flow, global radiation, soil temperatures, albedo and wind speed collected at the EFU level by means of the sensor clusters, and (c) air-borne thermal remote sensing that yields spatially highly resolved data on canopy/leaf temperature and soil surface temperature at different time slices during fair weather conditions. Basin scale spatial patterns of land cover and leaf area index are derived from Landsat and Modis satellite images.

Spatiotemporal variability of rainfall is characterized by merging operational rainfall radar data with ground based observations. These consist of the rain gauge data collected at the cluster locations, as well as distrometer data to characterize droplet sizes and vertical rain radar to correct vertical reflectivity profiles from three meteo-sites setup in the Attert basin. These data sources are combined along two avenues: (a) by means of data-assimilation into the soil-vegetation-atmosphere model system WRF-NOAH-MP (Samrock et al., 2008; Niu et al., 2011; Schwitalla and Wulfmeyer, 2014) (b) by a geo-statistical merging originally propose by Ehret (2002) to improve Quantitative Precipitation Estimates. Particularly promising is the assimilation of data

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of the new European polarization radar network, as this contains additional information concerning the size distribution of hydrometeors.

4.2 Blueprint of the CAOS model framework

4.2.1 Object structure and dimensionality of the flow problem

The CAOS model will be a parsimonious but still thermodynamically consistent model approach for simulating behavior of intermediate scale catchments, which allows also to test the value of organizing principles. Our key idea for balancing complexity and simplicity is to treat only the dominant processes determining the operative dominance of either EFUs or lead topologies in an explicit manner and to represent the hierarchy of these functional units by a hierarchy of coupled model objects which operate at different scales. Vertical and lateral flows of water, heat and solutes thus operate in separate process domains. This avoids solving of partial differential equations in several dimensions and minimizes the related computational burden and numerical challenges when using implicit numerical schemes. It allows a thermodynamic consistent treatment of the water, heat and matter balance in the different model objects. We furthermore propose that the model framework should optionally be able to account for dynamics of ecosystem engineers and vegetation because this creates feedbacks on soil structures and transpiration during non-stationary conditions (e.g. Schneider and Schröder, 2012).

4.2.2 Concepts for energy exchange and green water supply in the EFU domain

EFUs are the least model entities characterized by a surface/vegetation process domain and the unsaturated soil process domain (Fig. 7). During radiation driven conditions EFU operate in parallel sustaining energy exchange with the atmosphere; lateral mass exchange in the unsaturated soil matrix is neglected. As EFU class members are from the same ensemble, they are under ergodic conditions statistically homogenous with respect to the controls of the energy balance and related vertical fluxes of green water and heat. We thus suggest that one dimensional vertical treatment with explicit treatment of vertical preferential flow in wetting structures, as sufficient – not to reproduce the rich dynamics at the EFU scale and smaller scales – but to represent their controls on the energy balance and its relevant spatial variability at the intermediate scale of organized complexity. A 1-D vertical treatment implies that lateral variability of matric potential during radiation driven conditions be neglected (Zehe et al., 2006; Vogel and Ippisch, 2008; de Rooij, 2009). We suggest this is feasible up to a scale of 25 by 25 m^2. In the following we briefly present our first guesses for process representations at the EFU level.

Starting point for describing SVAT processes in the surface/vegetation domain is the Vegetation Optimality Model (VOM) (Schymanski, 2007; Schymanski et al., 2009). VOM is based on the hypothesis that vegetation adapts its degrees of freedom optimally to its environment in order to maximise its Net Carbon Profit (NCP) in the long term. Coupled water, heat and tracer budget during radiation driven conditions will be described by the one dimensional Richards, heat balance and convection dispersion equations. Root uptake will be implemented as in VOM. The key challenges at this scale are the assessment of effective soil water characteristics and representation of vertical preferential flow. A straightforward solution for the second problem is certainly a double permeability approach originally suggested by Beven and Germann (1981). A more visionary idea is a Lagrangian approach, based on water particles that carry heat and dissolved solute mass (Jackisch et al., 2013). Robust information on the topology of the vertical macropore network will arise from ecological survey and species distribution models for key ecosystem engineers such as earthworms, moles and voles (Schröder, 2008; Palm et al., 2013). Overland flow formation at the surface of the unsaturated soil domain is treated by means of a Cauchy boundary condition.

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4.2.3 Concepts for lateral flows and stream flow generation in hillslope scale lead topologies

We postulate that subsurface lateral exchange among EFU and lateral stream flow contribution is dominated by lateral preferential flow in drainage structures (Weiler and McDonnell, 2004; Wienhöfer and Zehe, 2014) and neglect lateral water flows in the unsaturated soil matrix (Fig. 7). Lateral preferential exchange between EFUs can be described in a one superordinate preferential flow network, which connects EFU objects downslope either at the surface or in the subsurface, and can meander in one or two dimensions (Fig. 7). This is inspired by the way we treat river flow in surface hydrology, because the river network comprises the preferential flow network in the catchment. These superordinate networks are additional objects at the hillslope domain, which is also characterized by a shallow aquifer system that extends down slope, controlling base flow production.

For subsurface pipe flow we assume (a) quasi steady state conditions i.e. the hydraulic gradient as parallel to slope in the pipe element, (b) that lateral flow starts when local saturation exceeds field capacity in a connected EFU object, and (c) exclusively unidirectional flow, employing the flow law of Darcy–Weisbach. Residence times of water and tracers within this lateral preferential flow domain depend on the number of EFUs connected to a pipe, the flow resistance in the pipe as well as the network topology. The proposed approach will be used to explore the link between network topologies, flow resistance in the superordinate network and bedrock slope on the shape of the residence time distribution. This insight will serve as a blueprint for defining typical topologies that cause typical shapes of the residence time distribution.

Overland flow is treated as a diffusion wave in a superordinate flow domain at the surface. By selecting a suitable topology we may either account for sheet flow (with parallel rills that are connected to each EFU within a lead topology) or for flow and transport in rills with a tree-shaped structure. Water levels in the rill network determine the pressure head that controls infiltration for the Cauchy boundary condition.

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4.2.4 Catchment scale model objects and free flow of blue water

Lead topologies are connected by the river net, which can be, depending on the geological setting, connected to deep aquifer systems. The river reach can be, depending on Strahler Order, connected to a riparian zone that connects to the hillslope. These are additional model objects that act at the highest scale level, the catchment domain. Coupled water, energy and mass transport in the shallow aquifer is described by the one dimensional Darcy law, heat transfer and convection dispersion equation. For the shallow aquifer we assume the dominant process directions as hillslope parallel. Exchange with the river system will be addressed by a leakage boundary condition; groundwater upstream in direction of the river will be treated with a diagnostic approach at a suitable time step. Water and energy flows in the channel domain will be accounted for by 1-D river hydraulics coupled with the energy balance equation as suggested for REWASH by Zhang and Savenije (2005) and Mou et al. (2008), or as proposed by Westhoff et al. (2007).

5 Concluding remarks

We expect our outlined experimental strategy to shed light on the question whether spatial organization in intermediate scale catchments is reflected by the existence of functional units which control the land surface energy exchange and event scale stream flow generation in different contexts. A key issue related to this, which is not discussed in this manuscript, is how to find the appropriate metrics for assessing similarity from geostatistics, graph-theory, mathematical morphology and multivariate statistics. The other key benchmark for the proposed concept is transferability of acceptable model parameter sets among members of the same EFU or lead topologies.

Even if we fail in corroborating the existence of functional units we expect that the CAOS project will foster a protocol to decide “where to assess which data for what reasons”, which will bring new momentum into our observations and understanding of

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links between landscape structure, distributed dynamics and integral flows in intermediate scale catchments. We put special emphasis on the explanatory value of different data sources added to this puzzle in order to work out the minimum necessary amount of field work to characterize structure-process interaction in intermediate scale catchments.

We are also convinced that the CAOS model concept will enable us to predict the interplay of distributed dynamics and integral behavior. The suggested model structure is sufficiently flexible to allow integration of various data sources characterizing soil texture, storage volumes, preferential flow paths as wells as surface and subsurface topography. We will compare the CAOS model performance against other types of hydrological models (LARSIM, Drogen, mHm). In this exercise we will put special emphasis on the value that different non-standard data sources provide for reducing model structural uncertainty.

The fact that spatial organization in catchments persists inspired many scientists to speculate whether this is a manifestation of self-reinforcing co-development due to an underlying organizing principle. The CAOS data set will allow us to test candidate organizing principles, which have been tested in neighboring scientific fields, and assess their explanative and predictive value in intermediate scale catchments. Special emphasis is on the development of test cases to assess the value of organizing principles for parameterizing dynamic fingerprints of subscale structure, for reducing equifinality and for making non-calibrated predictions.

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Table 1. Hierarchy of proposed functional classification scheme, affected catchment function, dominant similarities and related preferential flow path, as well as hydrological context of dominance.

Hierarchy level	Catchment function	First order controls with respect to similarities	Preferential flow path	Dominance
Geomorphic setting (catchment scale)	Blue water storage, base flow	Parent rock for soil formation, aquifer, geomorphology	River network	Permanent, long term
Lead topology (hillslope scale)	Stream flow generation & blue water supply	Potential energy differences: surface & bedrock topography, catena, aspect	Vertical and lateral macropore network	Rainfall driven conditions
EFU (pedon scale)	Energy exchange related green water & heat fluxes	Slope position & aspect, landuse, plant albedo, soil texture & hydraulic properties	Vegetation, network of biopores	Radiation driven conditions

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Table 2. Distribution of sensor clusters with respect to the characteristics of the corresponding functional units.

sensor cluster	north facing	south facing	slope position	near stream	plateau	forest	pasture
A			down			×	
B		×	mid			×	
C	×		mid			×	
D	×		up			×	
E	×		mid			×	
F			down	×		×	
G		×	mid			×	
H		×	up			×	
I					×		×
J				×			×
K		×	up				×
L		×	down	×			×
M		×	mid			×	
N			down	×		×	
O	×		mid			×	
P					×		×
Q		×	up				×
R		×	down	×			×
S		×	up			×	
T			mid			×	
U		×	down	×		×	
V	×		down	×		×	
W	×		mid			×	
total #	6	10		7	2	16	7

Discussion Paper | Discussion Paper | Discussion Paper | Discussion Paper |
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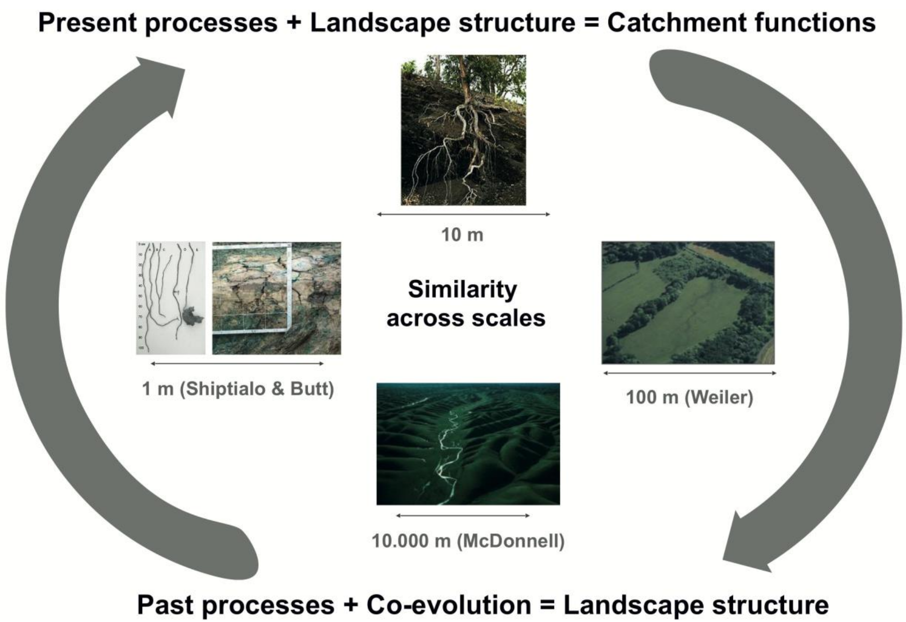

Fig. 1. "Drainage networks" that operate at different spatial scales and have been formed by different "agents". Starting clock wise at 9 o'clock: earthworm burrow network (Shipitalo and Butt, 1999, their Fig. 3.1) and crack network, root network, lateral rill network at grassland hillslope (photo by Marks Weiler) and the river network (photo by Jeff McDonnell).

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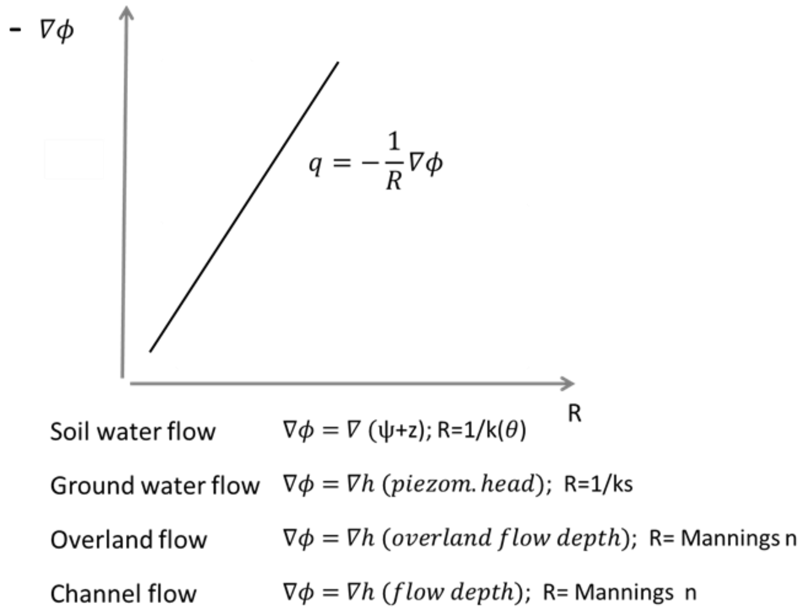

Fig. 2. Scheme of all combinations of potential gradients $\overrightarrow{\nabla\phi}$ and resistances R that compose the same flux q. Note that flow resistances in environmental systems control volume properties rather than material properties and are thus reduced by an apparent drainage network. In soil and for vegetation they non-linearly depend on system states. An increase in bedrock topography can for instance be compensated by decreasing subsurface transmissivity/hydraulic conductivity (i.e. increasing flow resistance) to maintain the same subsurface water flux.

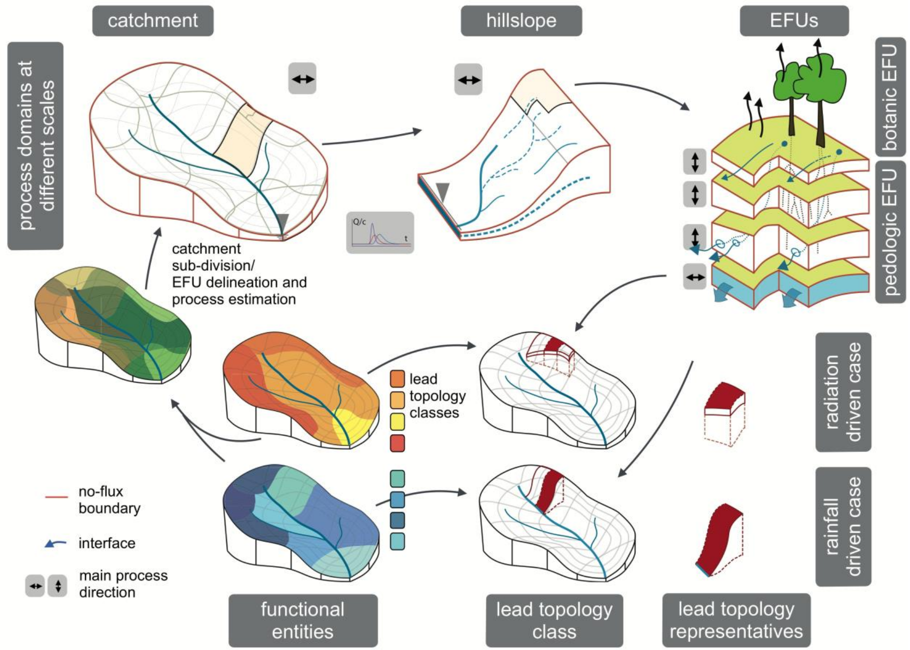

Fig. 3. Catchment functioning reflecting dynamic controls of different EFU or lead topologies. Members of the EFU compile similar surface energy balance, members of the same lead topology class compile a similar stream flow generation, when being in similar states and exposed to similar radiation/rainfall forcing.

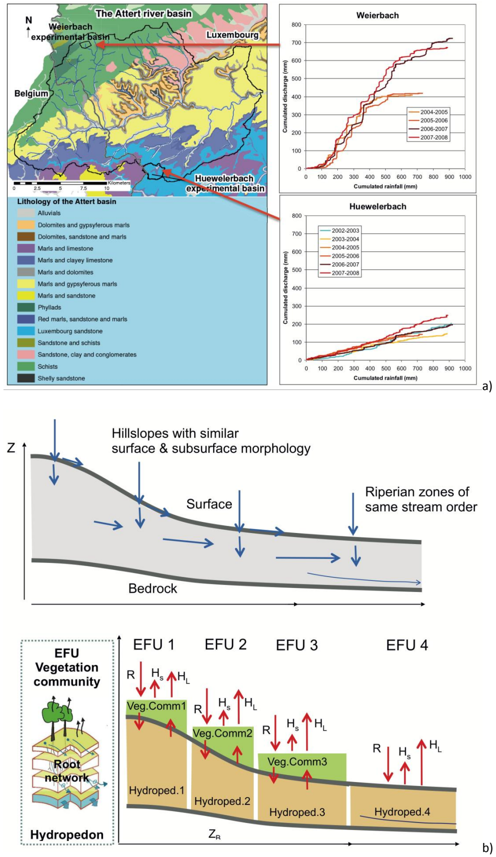

Fig. 4. Geology of the Attert basin as well as annual plots of accumulated discharge against accumulated rainfall for the Weierbach headwater, located entirely in Schist, and the Huewellerbach located in sandstone **(a)**. Scheme of lead topology and embedded elementary functional units controlling rainfall runoff response and land atmosphere energy exchange **(b)**.

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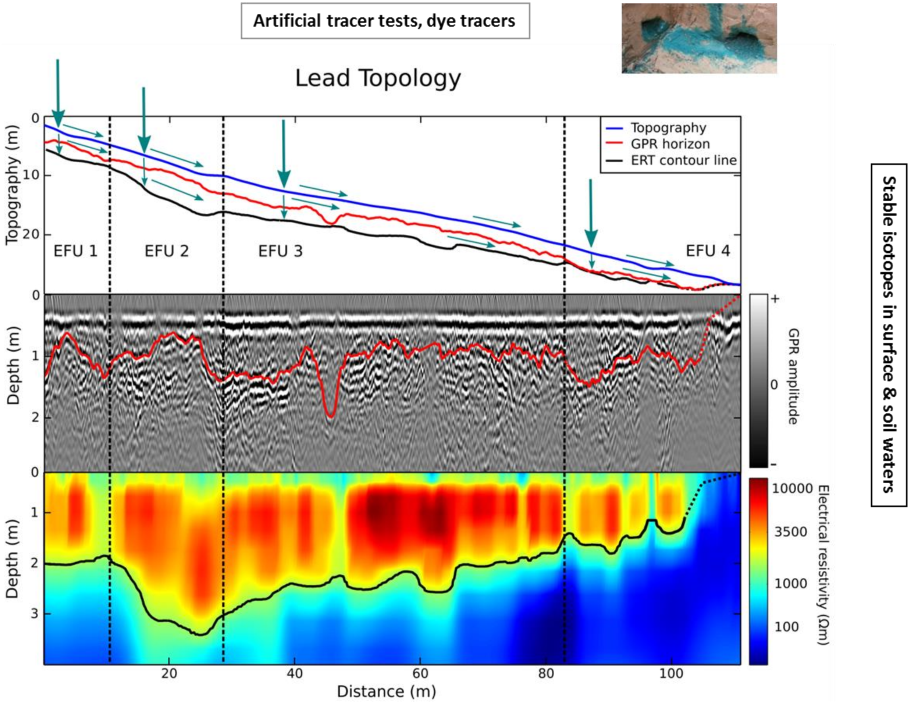

Fig. 5. Scheme outlining mutli-method approach to characterize first order controls on gradients driving lateral water flow as well as fingerprints of preferential flow in drainage networks.

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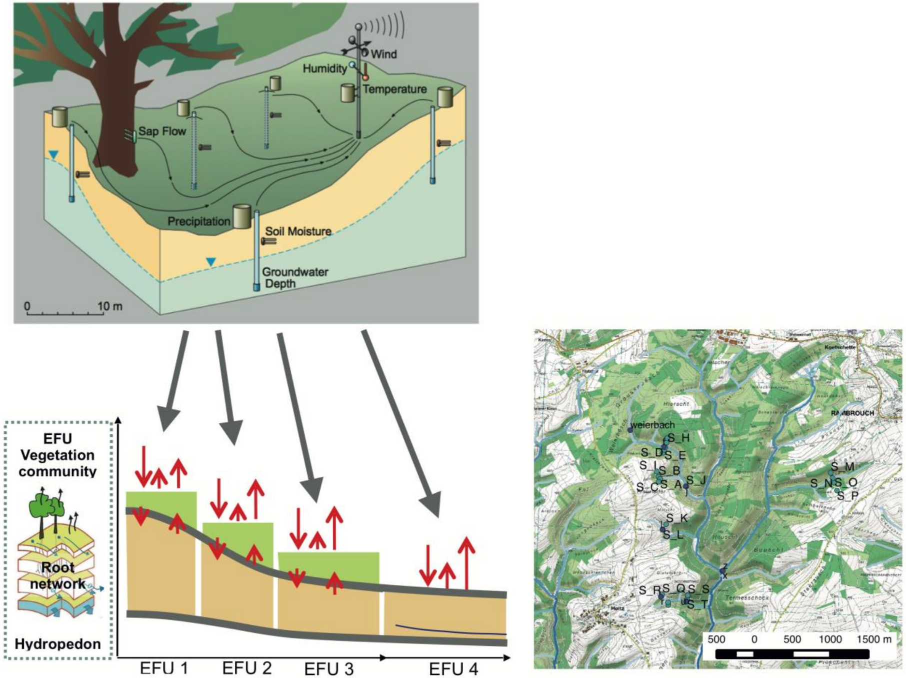

Fig. 6. Scheme outlining the multi-method approach to characterize EFU (left panel) within lead topologies by means of sensor clusters; distribution of sensor cluster in the Colpach (right panels red dots).

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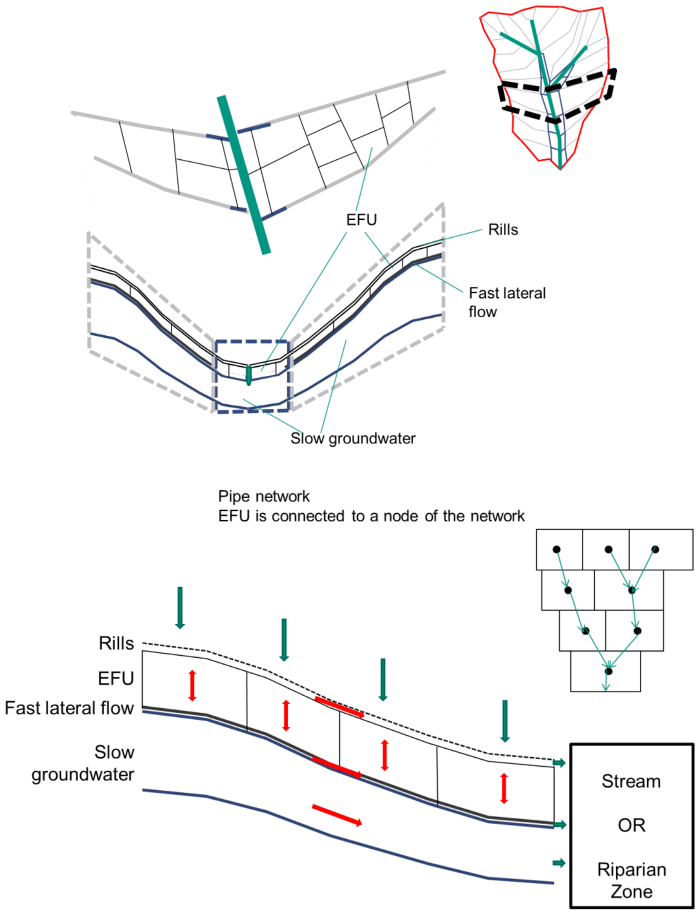

Fig. 7. Top panels: map view on catchment with EFU, water shed boundary and river net. Lower panels Arrangement of EFUs and their lateral exchange within the hillslope domain of proposed model structure of minimum necessary complexity.