From Catchments as Organised Systems to Models Based on Functional Units

Final Report –
Subproject F "Linking landscape structure and rainfall runoff behaviour in a thermodynamic optimality context" (CAOS Phase II) and
Subproject I "From subsurface structures to functions and texture - linking virtual realities and experiments at the plot and hillslope scales" (CAOS Phase I)

1 General Information

1.1 DFG reference number

ZE 533/12-1 Subproject Project F and ZE 533/8-1 Subproject I FOR1598

1.2 Applicant

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1.3 Topic

Phase II subproject F: Linking landscape structure and rainfall runoff behaviour in a thermodynamic optimality context;

Phase I project I. From subsurface structures to functions and texture - linking virtual realities and experiments at the plot and hillslope scales

1.4 Report- and Funding period

01.02.2012 - 31.12.2019

1.5 List of the most relevant publications

a) Peer-reviewed journal articles – first authors

Zehe, E., Loritz, R., **Jackisch, C.**, Westhoff, M., Kleidon, A., Blume, T., Hassler, S. K. and Savenije, H. H. (2019): Energy states of soil water – a thermodynamic perspective on soil water dynamics and storage-controlled streamflow generation in different landscapes, Hydrol. Earth Syst. Sci., 23(2), 971–987, doi:10.5194/hess-23-971-2019.

Zehe, E., and **C. Jackisch** (2016): A Lagrangian model for soil water dynamics during rainfall-driven conditions, *Hydrol. Earth Syst. Sci.*, *20*(9), 3511–3526, doi:10.5194/hess-20-3511-2016.

Jackisch, C., L. Angermann, N. Allroggen, M. Sprenger, T. Blume, J. Tronicke, and **E. Zehe** (2017): Form and function in hillslope hydrology: in situ imaging and characterization of flow-relevant structures, *Hydrol. Earth Syst. Sci.*, *21*(7), 3749–3775, doi:10.5194/hess-21-3749-2017.

Jackisch, C. and **Zehe, E.** (2018): Ecohydrological particle model based on representative domains, Hydrol. Earth Syst. Sci., 22(7), 3639–3662, doi:10.5194/hess-22-3639-2018.

Jackisch, C., Knoblauch, S., Blume, T., **Zehe, E.,** and Hassler, S. K. (2020): Estimates of tree root water uptake from soil moisture profile dynamics, Biogeosciences, 17, 5787-5808, 10.5194/bg-17-5787-2020.

Loritz, R., Kleidon, A., **Jackisch, C.**, Westhoff, M., Ehret, U., Gupta, H. and **Zehe, E.** (2019): A topographic index explaining hydrological similarity by accounting for the joint controls of runoff formation, Hydrol. Earth Syst. Sci., 23(9), 3807–3821, doi:10.5194/hess-23-3807-2019.

Loritz, R., Hassler, S. K., **Jackisch, C.**, Allroggen, N., van Schaik, L., Wienhöfer, J. and **Zehe, E.** (2017): Picturing and modeling catchments by representative hillslopes, Hydrol. Earth Syst. Sci., 21(2), 1225–1249, doi:10.5194/hess-21-1225-2017.

Loritz, R., Gupta, H., **Jackisch, C.**, Westhoff, M., Kleidon, A., Ehret, U. and **Zehe, E.** (2018): On the dynamic nature of hydrological similarity, Hydrol. Earth Syst. Sci., 22(7), 3663–3684, doi:10.5194/hess-22-3663-2018.

b) Peer-reviewed journal articles – co-authored

Allroggen, N., **Jackisch C.**, and Tronicke J. (2017): Four-dimensional gridding of time-lapse GPR data, pp. 1–4, IEEE. doi:10.1109/IWAGPR.2017.7996067

Angermann, L., **C. Jackisch**, N. Allroggen, M. Sprenger, **E. Zehe**, J. Tronicke, M. Weiler, and T. Blume (2017): Form and function in hillslope hydrology: characterization of subsurface flow based on response observations, *Hydrol. Earth Syst. Sci.*, *21*(7), 3727–3748, doi:10.5194/hess-21-3727-2017.

Glaser, B., **C. Jackisch**, L. Hopp, and J. Klaus (2019): How Meaningful are Plot-Scale Observations and Simulations of Preferential Flow for Catchment Models? *Vadose Zone Journal*, *18*(1), 180146 , doi:10.2136/vzj2018.08.0146.

Keller, S., F. M. Riese, N. Allroggen, **C. Jackisch**, and S. Hinz (2018): Modeling Subsurface Soil Moisture Based on Hyperspectral Data: First Results of a Multilateral Field Campaign, vol. 37, pp. 34–48, Deutsche Gesellschaft für Photogrammetrie, Fernerkundung und Geoinformation, München.

Malicke, M., Hassler, S. K., Blume, T., Weiler, M., and **Zehe, E**. (2020): Soil moisture: variable in space but redundant in time, Hydrology and Earth System Sciences, 24, 2633-2653, 10.5194/hess-24-2633-2020.

Reck, A., **Jackisch, C.**, Hohenbrink, T. L., Schröder, B., Zangerlé, A., van Schaik, L. (2018) ; Impact of Temporal Macropore Dynamics on Infiltration: Field Experiments and Model Simulations. Vadose Zone J, 17:170147.

Schneider, A. K., Hohenbrink, T. L., Reck, A., Zangerle, A., Schroder, B., **Zehe, E.**, and van Schaik, L. (2018):

Variability of earthworm-induced biopores and their hydrological effectiveness in space and time, Pedobiologia, 71, 8-19, 10.1016/j.pedobi.2018.09.001.

Seibert, S. P., **C. Jackisch**, U. Ehret, L. Pfister, and **E. Zehe** (2017): Unravelling abiotic and biotic controls on the seasonal water balance using data-driven dimensionless diagnostics, *Hydrol. Earth Syst. Sci.*, *21*(6), 2817–2841, doi:10.5194/hess-21-2817-2017.

Sternagel, A., **R. Loritz**, W. Wilcke, and **E. Zehe** (2019): Simulating preferential soil water flow and tracer transport using the Lagrangian Soil Water and Solute Transport Model, *Hydrol. Earth Syst. Sci.*, *23*(10), 4249–4267, doi:10.5194/hess-23-4249-2019.

Sternagel, A., **Loritz, R.**, Klaus, J., Berkowitz, B., and **Zehe, E.** (2021): Simulation of reactive solute transport in the critical zone: a Lagrangian model for transient flow and preferential transport, Hydrology and Earth System Sciences, 25, 1483-1508, 10.5194/hess-25-1483-2021.

c) Other Publication

In line with the DFG guidelines, we omitted explicit listing of posters and oral presentation at international workshops and conferences.

d) Patents

None

2 Final progress report

2.1 Project's initial questions and objectives

The main objective of project F was to explore an alternative thermodynamic perspective on hydrological dynamics by addressing the following research questions:

- To which extent can the interplay of preferential flow and rainfall-runoff in different soil landscapes be predicted based on thermodynamically optimal model structures? Can we, in case of biotic macropores, understand the benefit for ecosystem engineers from a co-evolutionary perspective?
- Does an apparent disequilibrium in landscape structure (reflected in topography, vegetation pattern, soil catena and apparent preferential pathways) imply temporally persistent patterns of soil moisture states in the sense that they 'mirror image' apparent disequilibria in the landscape and thus coincide nevertheless with local thermodynamic equilibria? If so, can this be explored for useful predictions of distributed state dynamics?
- Can we re-define hydrological similarity with respect to free energy stocks and conversions related to rainfall-runoff instead of focusing directly on the mass balance? If so, is this helpful to classify larger landscape control volumes (catchments and hillslopes/ lead topologies as defined in the framework document) with respect to their behaviour?

We planned to address these questions by testing three hypotheses:

- **H1:** Hydrological dynamics cause oscillations of soil moisture states around a local thermodynamic equilibrium pattern, which is determined by topography, soil pattern and related soil water retention properties, vegetation, density of preferential pathways and ground and surface water levels. Rainfall-runoff and related soil water dynamics happen in two different dynamic regimes (c- or p-regime), which can be characterized by a dimensionless number defined as the ratio of temporally averaged changes in capillary binding energy and potential energy associated with soil wetting and soil water flow. This dimensionless number depends on the climate and the above-listed landscape characteristics.
- **H2:** The potential natural state of the critical zone in the terrestrial system is organized such that it maximizes either steady-state net reduction (export and dissipation) of free energy during rainfall runoff in the c-regime or approaches an energetic steady state in the p-regime. This implies a) the opportunity for uncalibrated predictions and b) a certain possible diversity in “architectures” of the critical function which function in an optimal sense. The benefit for biota is a minimized disturbance regime due to an on average fastest relaxation back to local thermodynamic equilibrium, and possibly an increased resilience against “hydro-mechanical” disturbances. Ecosystem engineers in the c-regime (characterized by cohesive soils) benefit in particular by minimization of dry stress in summer due to moist but drained conditions and which maximizes the period they can stay active, as they get dormant during dry conditions (van Schaik et al. 2013).
- **H3:** Functional similarity of lead topologies and catchments during rainfall should not be defined based on similar stocks of water and runoff (mass export to the stream) but based on the storage, export and dissipation of free energy (power) during rainfall-runoff. Due to H2, this implies the opportunity to predict steady-state power P [J $m^{-2}s^{-1}$]/free energy export of lead topologies and to infer from this on steady runoff contributions and thus annual runoff coefficients.

2.2 Project developments and conducted research

During the second funding period, we tested and confirmed hypothesis H1 (Zehe et al. 2019) and H3 (Loritz et al.; 2019; Zehe et al. 2019), and derived other measures of functional similarity (Seibert et al. 2017) as briefly explained in sections (2.2.1).

Instead of testing H2, stating that a thermodynamic optimality model structure allows uncalibrated predictions, we focused on testing the central CAOS hypothesis postulating the existence of functional units of similar hydrological behaviour (Zehe et al., 2014). The studies of Loritz et al. (2017, 2018) confirmed the existence of functional units for runoff generation at the hillslope scale as detailed in section 2.2.2

Furthermore, we successfully advanced research activities started within the first funding Phase within Project I 'From subsurface structures to functions and texture linking virtual realities and experiments at the plot and hillslope scales (ZE 533/8-1)'. This includes firstly a detailed soils survey and characterisation of preferential flow activities using dye tracers and new ways for in-situ imaging of rapid subsurface flow by combining time-lapse ground-penetrating radar with TDR profiling (Jackisch et al., 2017). Secondly, we have develop a Lagrangian model framework for simulating soil water dynamics in heterogeneous soils (Zehe and Jackisch, 2016) including macropores (Jackisch and Zehe, 2018). This avenue has been advanced through a recent development of a Lagrangian model for water and solute transport (Sternagel et al., 2019; Sternagel et al., 2020).

2.2.1 A thermodynamic perspective on soil water dynamics and runoff generation

Zehe et al. (2019) and Jackisch et al. (in prep) developed a new thermodynamic perspective on soil water dynamic dynamics, which is well suited to distinguish the typical interplay of gravity and capillarity controls on soil water dynamics in different landscapes. The idea is to express the driving matric and gravity potentials by their energetic counterparts and characterize the soil water content by its Gibbs free energy e_{free}:

$$de_{free} = \rho g \theta d\psi + \rho g \theta dz \quad \text{(Eq. 1)}$$

Where g (ms^{-2}) is gravitational acceleration, z (m) denotes the position in the gravity field, θ (m^3m^{-3}) the soil water content, ρ (kgm^{-3}) the density of water and ψ (m) the matric potential.

E_{free} reflects both the binding state and the amount of water that is stored in a control volume at a given elevation above groundwater and thus relates to the local retention properties and the topographic setting as well. Zehe et al. (2019) used free energy to define a new system characteristic determining the possible range of energy states of soil water named energy state function (Fig. 1). Note that in this state function, the soil water content at local equilibrium separates storages corresponding to positive and negative free energies ranges we call the P- and the C-regimes. Wetting of the soil beyond the equilibrium storage implies and excess in positive potential energy, corresponding to a state of a storage excess. We call this range the P-regime because potential energy and hence gravity acts as dominant driver for soil water dynamics. Relaxation back to equilibrium requires to release water e.g. in the form of runoff or seepage to deplete the excess in potential energy, and the necessary amount is determined by the overshoot of free energy above zero. Storages smaller than the equilibrium imply that negative capillary binding energy exceeds potential energy. We call this range the C-regime because capillarity acts as the dominant driver for soil water dynamics. The system needs to recharge water to replenish the "energy deficit" below zero, and the necessary amount depends on the distance to equilibrium. The energy state function defines the possible energy states of the soil water storage at a given point above groundwater. Due to the intermittent rainfall and radiative forcing, the free energy state of soil water will be pushed and pulled through this state space.

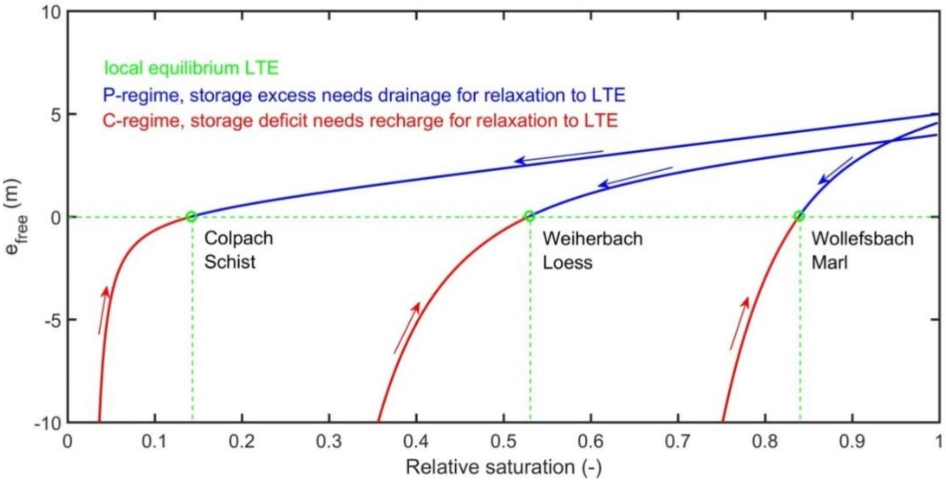

Figure 1: Weight specific free energy state of the soil water storage, plotted against the relative saturation of the three different soils, assuming a depth to groundwater of 10m. The green lines mark the local equilibrium state where the absolute value of the specific free energy is zero and the corresponding equilibrium saturations. Free energy in the P-regime and C-regimes are plotted in solid blue and red respectively, the arrows indicate the way back to equilibrium.

Figure 2 shows this exemplarily using pairwise soil moisture and matric potential data observed at in two different soils, which are both located 20 m above their respective streams.

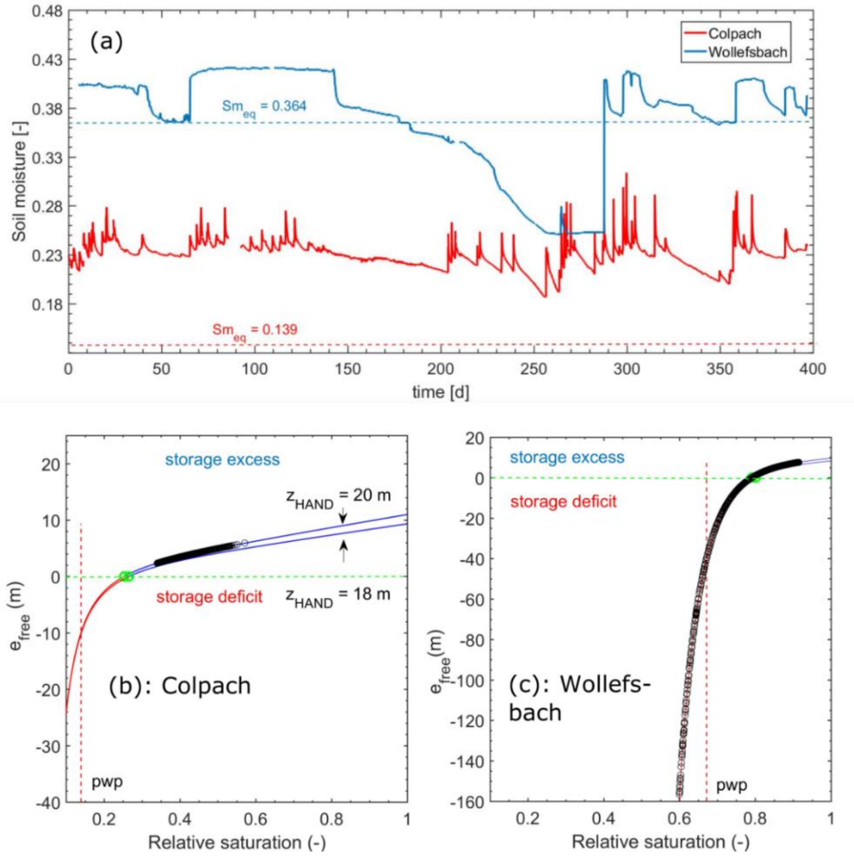

Figure 2: Topsoil water content observed at cluster sites in the Colpach and the Wollefsbach catchment (panel a) and the corresponding free energy states in their respective energy state curves (panel b and c note the different scaling of the ordinates). The black circles mark the observations. The vertical dashed line marks the permanent wilting point. Panels b and c show additionally the energy state curve when contamination the real value with an error of minus 2 m (z_{HAND} = 18 m).

The soil water content in the clay-rich topsoil of the Wollefsbach site is in the winter and fall period rather uniform and on average 0.15 m^3m^{-3} larger than in the Colpach (Fig. 2a). The soil water content at the Colpach site appears much more variable in these periods. Both sites dry out considerably during the summer period and start to recharge with the beginning of the fall. Figure 2a shows furthermore that the site in the Colpach operates clearly above the corresponding soil water content equilibrium, θ_{eq} = 0.139 m^3m^{-3}, while the site in the Wollefsbach drops below its soil water content equilibrium, θ_{eq} = 0.364 m^3m^{-3}, and operates in the C-regime for almost 3 months. Figure 2 b and c provide the corresponding free energy states of both soil water time series as a function of the soil saturation. The first thing to note is that the observed free energy states for both sites scatter nicely around the theoretical curves. One can also see that the spreading of the free energy state of the soil water stock is at both sites distinctly different. The free energy state of soil water at the Colpach site is during the entire hydrological year in the P-regime and hence subject to an overshoot in potential energy (Fig. 2 b). In the Wollefsbach the weight-specific free energy density of soil water spreads across a much wider range and most importantly, the system operates qualitatively differently as it switches to the C regime during the dry spell in the summer period and stays there for nearly three months. Zehe et al. (2019) reported similar findings for the entire distribution of soil moisture and matric potential observations in both test catchments. We thus state that these findings largely corroborate hypothesis H1.

The free energy state of soil water in the riparian zone of both study catchments provides furthermore a theoretical sound explanation of the threshold like the onset of streamflow generation (Fig. 3). We found a distinct threshold behavior for storage controlled runoff production in both catchments, and clear hints at Hortonian overland flow contributions in the Wollefsbach - the onset of a potential energy excess of soil water in the riparian zone coincides with the onset of storage controlled streamflow generation.

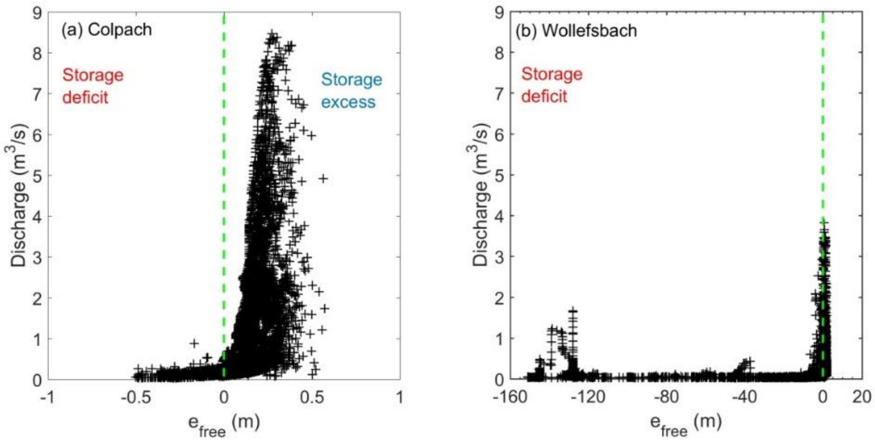

Figure 3: Observed stream flow in the Colpach (a, drainage area is 19.4 km^2) and the Wollefsbach (b, drainage area is 4.5 km^2) plotted against the free energy of sites in their corresponding riparian zones.

Complementary to that Loritz et al. (2019) proposed a novel thermodynamic index to better explain topographic controls on runoff generation. Given that potential energy differences are the main drivers for runoff generation, topography provides important information to explain runoff generation in catchments. However, due to the strongly dissipative nature of runoff generation, the driver of a flux explains only one aspect of the runoff generation. In fact, dissipative losses dominate runoff generation and even in case of overland flow only a tiny portion of the driving potential energy is transformed into the kinetic energy of runoff. We thus proposed a new topographic index named reduced dissipation per unit length (rDUNE), which jointly accounts for the energetic driver and the dissipative loss along the flow path. rDUNE allowed a superior discrimination of six catchments into groups of similar runoff generation than the often recommended height over next drainage (HAND) or the famous topographic wetness index (TWI).

Overall the findings reported in Zehe et al. (2019) and Loritz et al. (2019) corroborate that a thermodynamic perspective hydrological systems offer holistic information for judging and inter-comparing soil water storage and runoff generation, which cannot be inferred from the traditional water balance thinking alone.

2.2.2 From catchment as organized systems to dynamic hydrological similarity?

Within two related model studies Loritz et al. (2017, 2018) corroborated that hydrological landscapes can be divided into hillslope scale functional units, which in turn can be used as building blocks for setting up simplified and yet physically sound hydrological models. The first study showed that the water balance of the forested Colpach in the Devonian schist/slate (19.4 km2) and the agricultural Wollefsbach in the Marls (4.5 km^2), can successfully be simulated by a single 2d representative hillslope. The model parametrizations are based on the perceptional models of both landscapes derived from expert knowledge (Fig. 4). Moreover, they were largely informed by the available comprehensive field data on soil hydraulic properties, macropores (from project A). Particularly the geophysical data from project B were helpful to constrain the subsurface topography in the Colpach model.

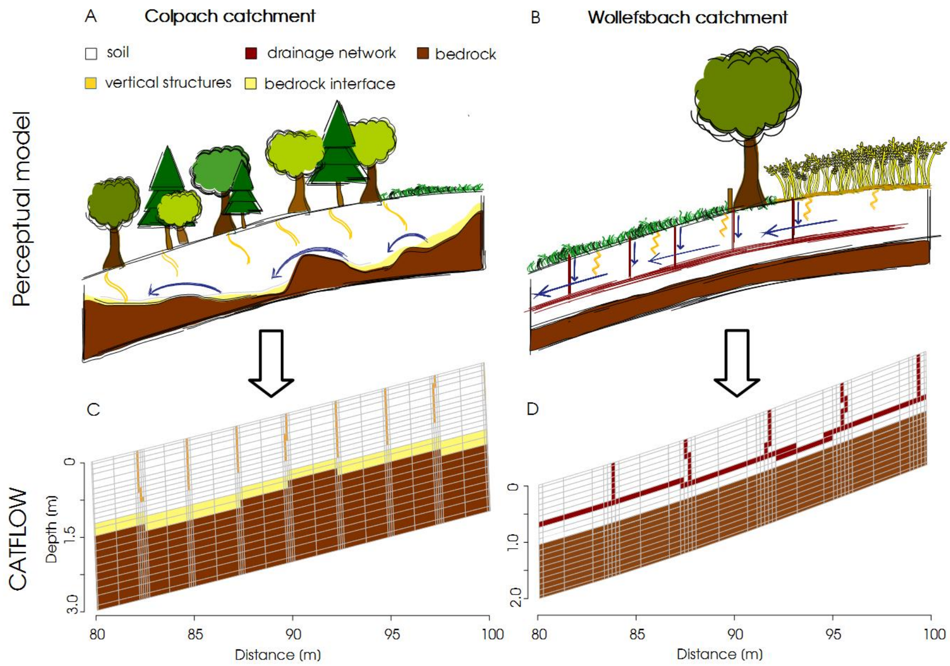

Figure 4: Perceptual models of the (a) Colpach and (b) Wollefsbach and their translation into a representative hillslope model for CATFLOW. It is important to note that only small sections of the model hillslope are displayed (C Colpach; D Wollefsbach).

The corresponding simulations of stream flow (Colpach KGE 0.88, Wollefsbach KGE 0.71), transpiration and distributed soil moisture dynamics were in both catchments in acceptable accordance with observations of the hydrological year 2013/14 (Loritz et al., 2017).

This underpins that the concept of representative hillslopes is a feasible approach to simplify distributed models without lumping, because they preserve the relevant information about the average driving gradients and resistance terms that control runoff generation and hydrological dynamics. The key to the derivation of these representative hillslopes this was to respect energy conservation during the aggregation procedure. Specifically, we derived an effective topography such that it conserved the average distribution of potential energy along the averaged flow path length to the stream. Similarly, the macroscale effective soil water retention curve was constrained to preserve the relation between the average soil water content and matric potential energy using the set point scale retention experiments (see section 2.2.3, Fig. 7). Test simulations with randomly selected retention functions of individual experiments and based on the averages of the individual parameter sets performed clearly worse (see CAOS synthesis report).

Along similar lines, Loritz et al. (2018) showed that simulations by means of a fully distributed setup of the same Colpach catchment using 105 different hillslopes yielded strongly redundant contributions of streamflow (Fig. 5). They used the Shannon entropy (Shannon, 1948) to quantify the diversity in the simulated runoff of the hillslope ensemble at each time step. Note that an entropy maximum implies that hillslopes contribute in a unique fashion, while a value of zero implies that all hillslope yield a similar runoff response. This revealed that the entropy of the runoff ensemble was rather dynamic in time but it never reached the maximum value, which implied that the hillslopes yielded strongly redundant runoff contributions to stream flow (Fig. 5c).

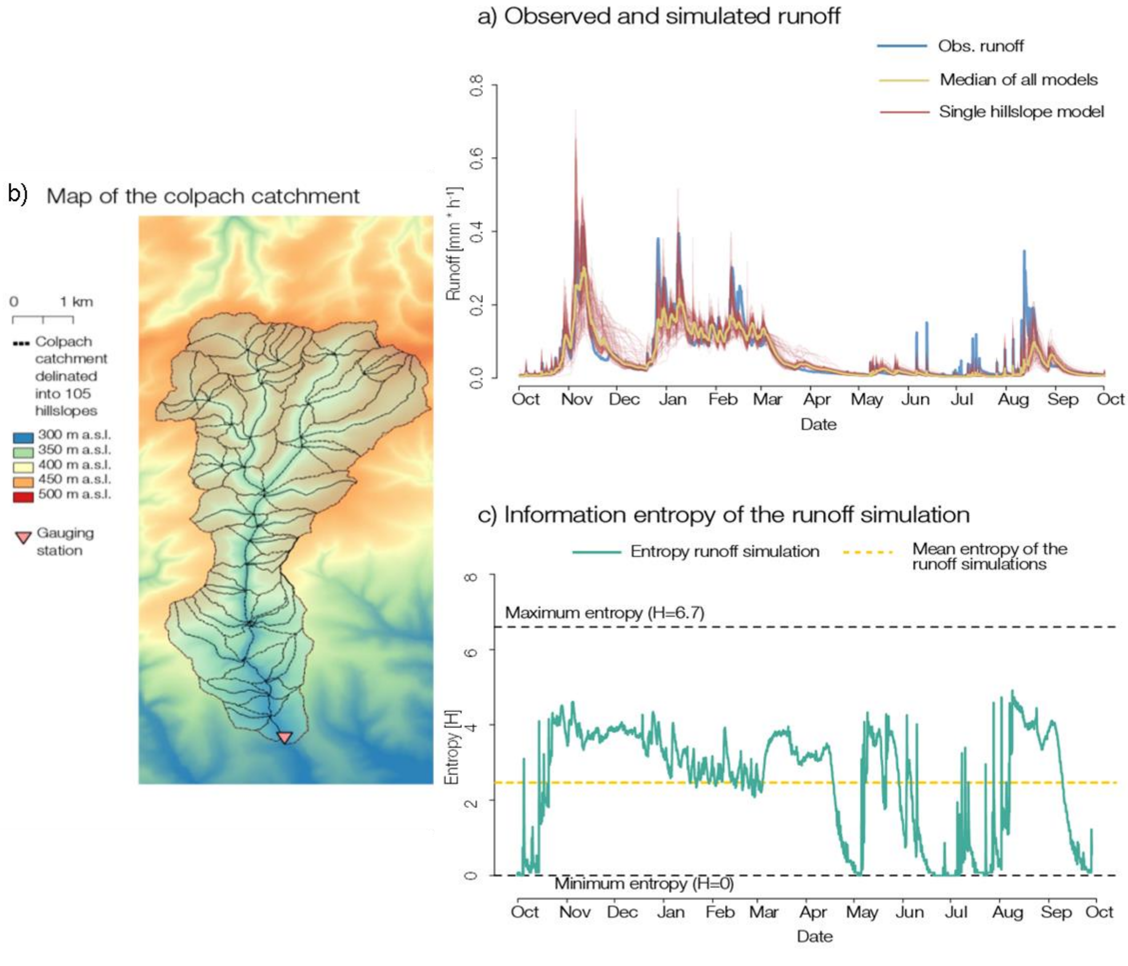

Figure 5: (a) Observed and simulated runoff of the Colpach catchment. The red lines correspond to individual hillslope models and the yellow line to the area-weighted median of all hillslopes. (b) Map of the Colpach catchment and the 105 different hillslopes. (c) Shannon entropy in turquoise for the runoff simulations as well as the corresponding mean. © Ralf Loritz KIT, from Loritz et al. (2018).

We further showed that the set of 105 hillslopes could be clustered into six functional units of similar runoff response based on their mutual information. When using scaled runoff simulations from six arbitrarily picked representatives of these functional units, their sum performed on average as good to the full ensemble as further detailed in Loritz et al. (2018).

We thus conclude fully distributed model could considerably be compressed without information and thus performance loss, thereby avoid redundant computations.

This finding corroborates the existence of functional units for runoff generation and it furthermore explains why conceptual models with 5-6 parameters simulate rainfall runoff behavior of catchment often very well, as most of the topographical heterogeneity in the catchment is irrelevant for runoff production. Recent studies yielded similar findings for a simple conceptual model (Ehret et al., 2020) and for CATFLOW when being used with gridded radar based rainfall estimates (Loritz et al., 2021).

2.2.3 Distributed survey of soils structures and preferential flow processes

In the first funding period, we investigated in close cooperation with phase I projects J and E the role of preferential flow paths by means of dye staining of flow paths and bromide tracer tests carried out at different irrigation intensities in all geological settings. This revealed a dominance of rapid flow with tracer travel depth of up to 2m within 1 day (Fig. 6). Moreover, we established a workflow to derive the soil water retention and unsaturated hydraulic conductivity curves using a large set of undisturbed soil cores from selected sites within all geological settings. This was combined with soil augers, constant head permeameter measurements and detailed soil type mapping in soil pits and dye staining (Jackisch et al., 2017).

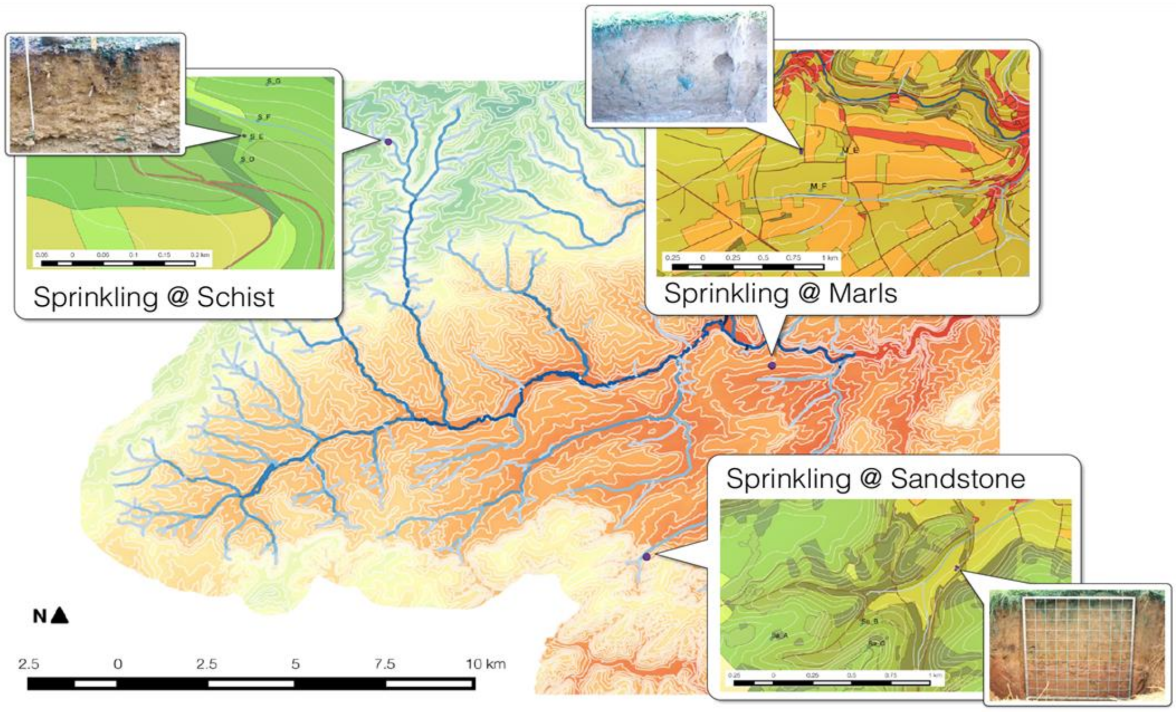

Figure 6: Map of Attert Basin and locations of Sprinkler Experiments

Overall, more than 120 soil cores were analysed for their retention properties and their saturated hydrologic conductivity. These data revealed that rapid flow in the silty soils in the Devonian slates operates within a well-connected network of inter-aggregate pores (Jackisch et al. 2017). Using this set of distributed retention experiments Jackisch et al. (2017) derived macroscale effective soil water retention curves (Figure 7) to sustain modelling efforts using representative hillslopes (Loritz et al., 2017) as detailed in section 2.2.2. Moreover, joint research with phase I project F revealed that laps GPR in combination with TDR profiling turned out to be a powerful combination to visualise and quantify vertical and lateral subsurface flows (Jackisch et al.; 2017; Allrogen et al., 2017, see CAOS synthesis report for more details).

2.2.4 Lagrangian modelling of water and solute transport in structured soils

The inability of the Richards equation to preferential flow in structured soils is well known. Although a range of approaches has been proposed to address this problem (Šimůnek et al., 2003; Beven and Germann, 2013) none of those are commonly accepted as superior. A novel avenue, which offers the assets of both double-domain and spatially explicit approaches are Lagrangian models. The Lagrangian perspective has been used up to now only to simulate advective-dispersive transport of solutes (Berkowitz et al., 2006). Lagrangian descriptions of the fluid dynamics itself are only realized in a few models namely SAMP (Ewen, 1996a, b), MIPs (Davies et al., 2013). Within the first funding period, we started to develop Lagrangian models for simulating soil water dynamics and solute transport in structured heterogeneous soils (Zehe and Jackisch, 2016; Jackisch and Zehe, 2018; Sternagel et al. 2019).

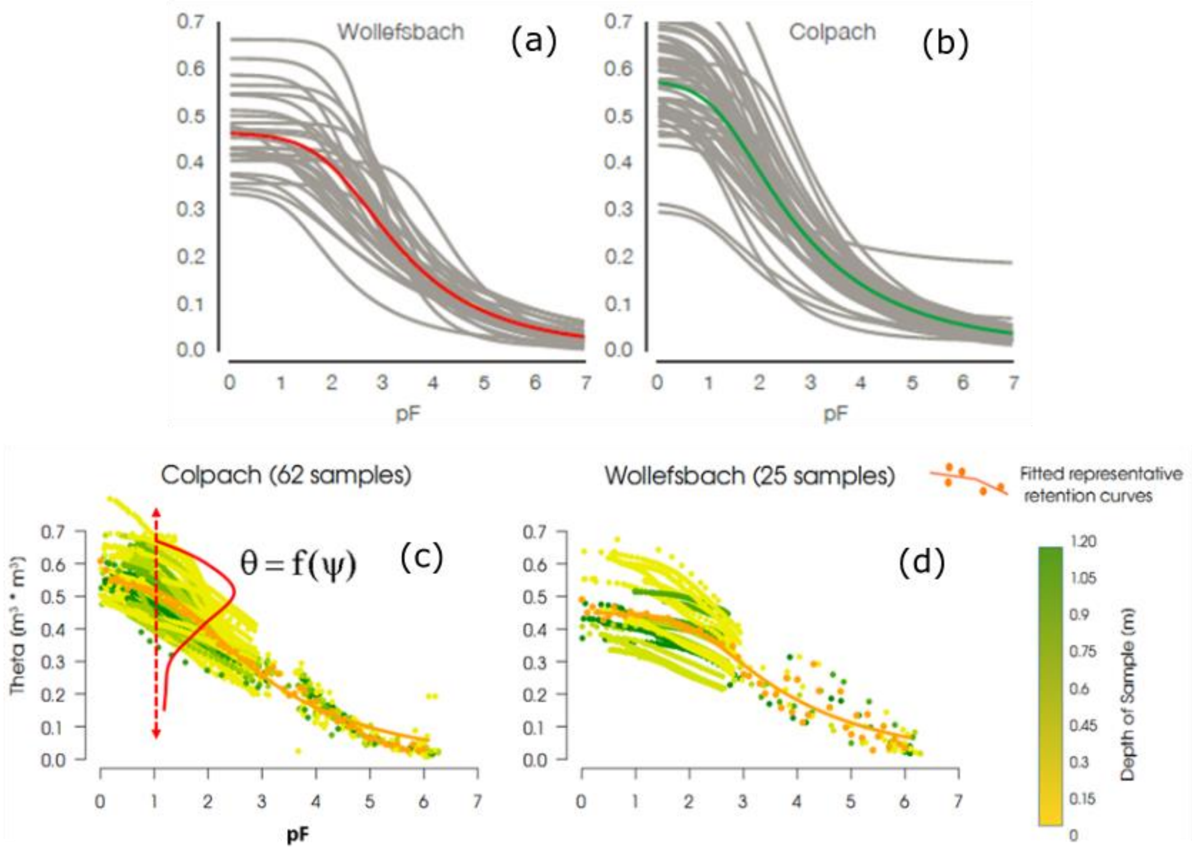

Figure 7: Retention functions Jackisch (2015) derived from individual soil cores by means of multistep outflow experiments (a and b). Panels c and d illustrate the procedure of pooling the soil water contents observed at given tension (pF = $\log_{10}(\psi)$) of all experiments into conditional random samples. The orange points mark the averaged soil water content values as function of the tension and the solid lines are the mark fitted van Genuchten functions. Note that these representative curves are shown in color in panel a and b as well. The color code of the individual data points in panel c and d relates to the depth of the sample below surface.

Zehe and Jackisch (2016) conceptualized the first version of a Lagrangian model describing soil water flow using a non-linear space domain random walk, motivated by the equivalence of the Fokker Planck equation and the diffusive form of the Richards equation. In line with Ewen (1996), their model estimates the diffusivity and the gravity-driven drift term of the random walk based on the soil water retention curve and the soil hydraulic conductivity curve. A naive random walk, which assumes all water particles to move at the same drift velocity and diffusivity, overestimated depletion of soil moisture gradients compared to a 1d Richards solver (Fig. 8). The solution to this was to account for variable velocities, as characterized by the shape of the soil hydraulic conductivity curve. Depending on the actual water content, the travel velocities of water particles are distributed accordingly using a suitable binning. Because of this, the Lagrangian model accounts per default for the distribution of flow velocity within different pore size of soil matrix. It allows for furthermore for a separated treatment of pre-event and event-water particles and non-equilibrium infiltration as detailed in Zehe and Jackisch (2016).

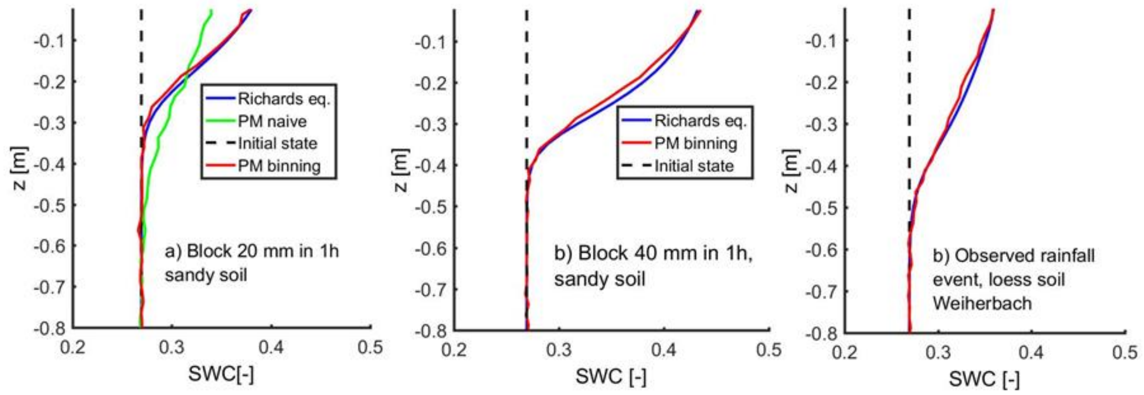

Figure 8: Soil moisture profiles simulated for a) a sandy soil and a block rain of 20 mm with a naive random walk (PM naive) and the Lagrangian particle model with binning (PM) according to Eq. 5 compared to a simulation with a Richards model, b) a sandy soil and a block rain of 40 mm, and c) an observed convective rainfall in the Weiherbach catchment.

This one dimensional approach was expanded by Jackisch and Zehe (2018) into a two dimensions using a structured domain containing macropores as one vertical dimensional explicit structures. Within those, the velocity of each particle is described by interactions of driving and hindering forces using a generalized Bernoulli equation (Fig. 9) following thermodynamic reasoning. The driver is the geopotential energy of a particle, while energy dissipation occurs due to frictional and capillary forces at the macropore walls. The assets of this new echoRD model are a (i) self-limiting film flow in macropores, (ii), the ability to simulate 2-D infiltration patterns based on (iii) observable parameters. The model has been proven capable to simulate non-uniform infiltration patterns in accordance with observed patterns and to explore related structural controls on travel distance distributions (Jackisch and Zehe, 2018). The model was also tested within different dynamic macropore settings in close cooperation with phase II project A (Reck et al., 2018). The results confirm the feasibility of echoRD to reproduce observed infiltration patterns (Fig. 10).

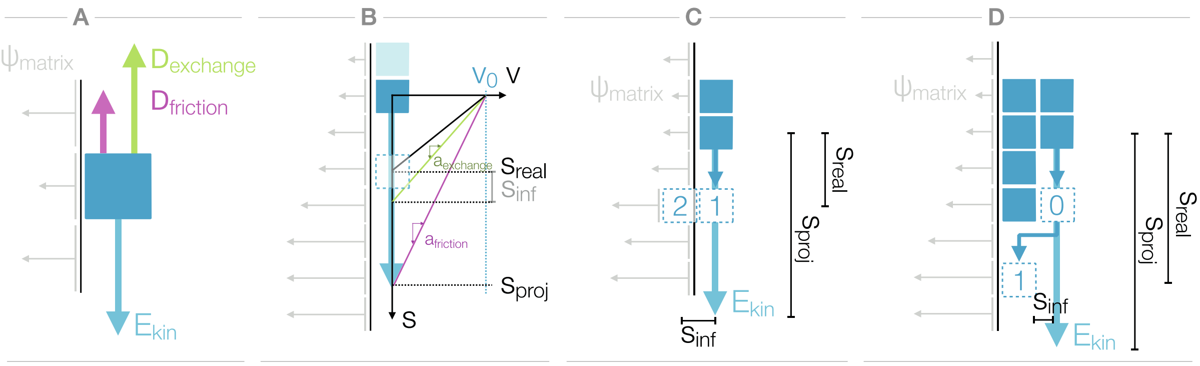

Figure 9: Macropore flow concept. (A) E_{kin} is dissipated by frictional and capillary forces at the macropore wall, (B) Projected advection with v_0 is decelerated, (C) possible infiltration if contact time exceeds infiltration time, (D) Fast advection of a particle as film flow until the end of the film.

Sternagel et al. (2019) generalized the Lagrangian approach to allow for simulations of water and solute transport in the matrix and a simplified separated macropore domain. Water particles are characterized by their location, mass and solute concentration. A size and depth distribution and hydraulic radius characterize the macropore domain. The latter is helpful to determine the fraction of particles having contact to the macropore-matrix interface. Flow in the macropore domain is purely advective and the related velocities can be inferred either from tracer data or from direct observations reported in the literature.

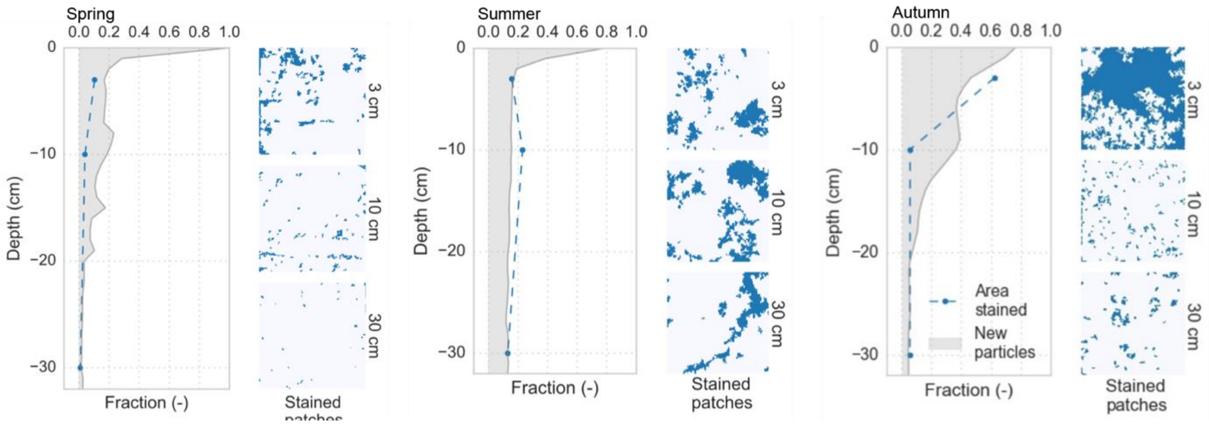

Figure 10: Observed staining in infiltration experiments at different seasons (blue) and modelled infiltration without calibration (grey).

The exchange water flux of pre-event water particles in the macropore domain with the surrounding matrix is calculated according to Darcy's law. Infiltration into the matrix and the macropores depends on their moisture state. A comparison of Hydrus 1d and the LAST-Model based on plot scale tracer experiments in the Weiherbach catchment revealed that both models show a similar good performance in case of matrix-flow-dominated tracer transport (Fig. 11, Hydrus 1d simulations are not shown). In case of preferential transport, LAST clearly outperformed Hydrus 1d (Sternagel et al., 2019). The macropore domain for this site was parameterized based on a local survey of the worm burrow system similar to those carried out in phase II project A. The corresponding flow velocities were calculated based on their cross sections, using a regression derived from flow experiments with undisturbed soil samples containing macropores of variable diameters.

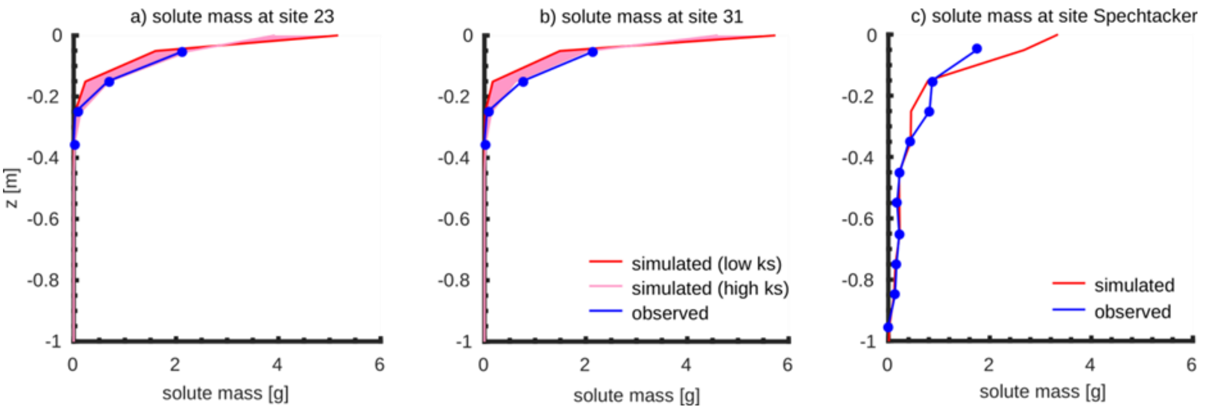

Figure 11: Final Lagrangian Soil Water and Solute Transport Model (LAST)-simulated and observed bromide mass profiles at two sites with dominant matrix flow (a, b) and a site with strong preferential transport (c), after irrigation with 10 mm/h for two hours. Shaded areas mark the uncertainty range caused by the uncertainty in observed hydraulic conductivity. Source: Sternagel et al., (2019).

The most recent version of LAST allows for simulation of reactive transport (Sternagel et al.; in review 2020). Transformation kinetics are simulated by transferring mass from the parent to the child component in each fluid particle according to the reaction rates, as each particle may carry concentrations of different substances. Respective concentrations are limited by the solubility. A retardation coefficient is not helpful in the particle-based framework, as the solute mass travels with the water particles and thus by default at the same velocity. LAST therefore accounts for a reduced solute mobility through explicit transfer of dissolved mass from the water particles at a given depth to surrounding adsorption soil sites (and vice versa). This may either operate under rate-limited or non-limited conditions. If the maximum concentration of the adsorbed substance is locally reached, the remaining solute will travel in a non-adsorbing manner. A first simulation of plot-scale Isoproturon transport observed at the same site in the Weiherbach catchment yielded promising results compared to simulations with Hydrus 1d (Fig. 12).

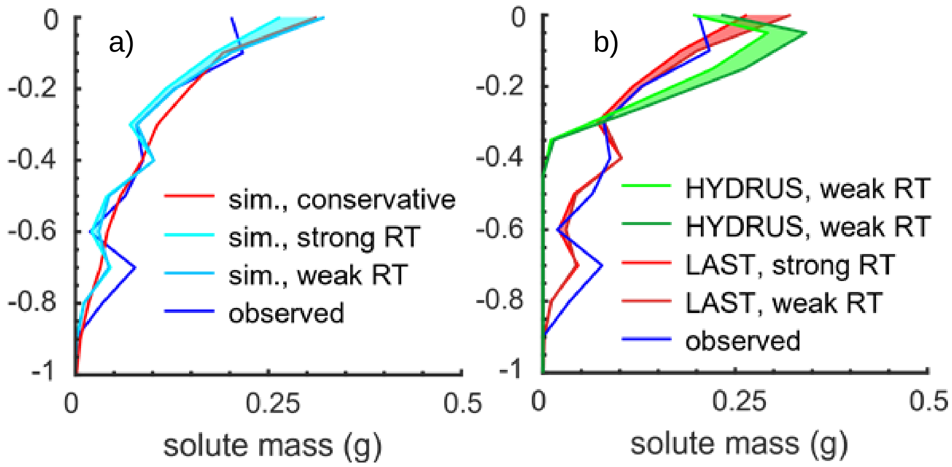

Figure 12: Simulated and observed Isoproturon profiles using LAST at a Weiherbach site dominated by preferential flow (Zehe and Flühler, 2001) 2 days after application (a), revealing differences in simulated conservative and different reactive transport parametrizations due to the variations of the KF and DT 50 values (RT). Benchmark simulations with Hydrus 1d, shaded areas illustrate the variations of the KF and DT 50 values (b). @ KIT, Sternagel et al. (2021).

All these findings corroborate that Lagrangian models provide many assets to simulate flow and transport in heterogeneous soils compared to the traditional Richards and Advection-Dispersion equations.

2.3 Qualification of young researchers in the context of your project

Dr. Conrad Jackisch and Dr. Ralf Loritz successfully finalized their Ph.D. theses within this project and received their doctorates from the department of Civil Engineering, Geo- and Environmental Sciences at the Karlsruhe Institute of Technology in 2015 and 2019. Dr. Jackisch has been recently appointed as Junior-Professor at the Technische Universität Bergakademie Freiberg. Moreover, the project provided food for MSc theses by Nina Kiese, Leonard Bartels, and Alexander Sternagel.

Moreover, we organized several summer and winter schools:

- 3 days winter school 2015 (March) Axel Kleidon, Erwin Zehe (Thermodynamics in Earth system science)
- 4 days summer school 2018 (March) Rui Perdigão (Dynamic System Analysis in Environmental Sciences)
- 2 days summer school 2018 (March) Axel Kleidon, Erwin Zehe (Thermodynamics in Earth system science)

3 Summary

This project explored, within the frame of the CAOS research unit FOR 1598, a new thermodynamic perspective on hydrological dynamics. To this end, Zehe et al. (2019) characterized the soil water content by its Gibbs free energy, which jointly reflects gravity and capillary controls. From this, they derived a new system characteristic determining the possible range of energy states of soil water, which is well suited to distinguish the typical interplay of gravity and capillarity controls on soil water dynamics in different landscapes. Moreover, the energy state functions consist of two different regimes associated either with a storage excess or with a storage deficit. Zehe et al. (2019) showed that storage dynamics into different landscaped is straightforwardly visualized as distinctly pseudo oscillations of the corresponding free energy state around the local equilibrium. The free energy state of soil water in the riparian zone of both study catchments provides furthermore a theoretically sound explain of the threshold like onset in streamflow generation. Complementary to that Loritz et al. (2019) proposed a novel thermodynamic index to explain topographic controls on runoff generation named reduced dissipation per unit length (rDUNE). rDUNE jointly accounts for the energetic driver and the dissipative loss along the flow path and a provided stronger discrimination of catchments into groups of similar runoff generation than HAND or the topographic wetness index (TWI).

Moreover, we corroborated the central CAOS hypothesis postulating the existence of functional units of similar hydrological behaviour (Zehe et al. 2014) within two related model studies (Loritz et al., 2017; 2018). The first study (Loritz et al. 2017) corroborated that the water balance of two different mesoscale catchments, the Colpach and the Wollefsbach, can successfully be simulated by a single 2d representative hillslope. In both catchments, the representative models yielded simulations of streamflow, optionally sap flow and distributed soil moisture dynamics in good accordance with observations. This success is explained by the fact that both models preserve the relevant information about the driving gradients and resistance terms that control runoff generation and hydrological dynamics. Furthermore, Loritz et al. (2018) showed by means of the Shannon entropy that simulations by means of a fully distributed setup of the same Colpach catchment using 105 different hillslopes yielded strongly redundant contributions of streamflow. They further showed that the fully distributed model, consisting of 105 hillslopes, could be compressed to a model using six hillslopes with distinctly different runoff responses, without a loss in simulation performance. In both catchments, the representative models yielded simulations of streamflow, optionally sap flow and distributed soil moisture dynamics in good accordance with observations.

Furthermore, we successfully advanced research activities started within the first funding Phase within Project I ‘From subsurface structures to functions and texture linking virtual realities and experiments at the plot and hillslope scales (ZE 533/8-1)’. This includes firstly new ways for in-situ imaging of rapid subsurface flow by combining time-lapse ground-penetrating radar with TDR profiling (Jackisch et al., 2017). Secondly, we started to develop Lagrangian models for simulating soil water dynamics and solute transport in structure heterogeneous soils (Zehe and Jackisch, 2016; Jackisch and Zehe, 2018, Sternagel et al., 2019). These studies underpin that Lagrangian models provide many assets to simulate flow and transport in heterogeneous soils compared to the traditional Richards and Advection-Dispersion equations.

Overall these findings corroborate that a thermodynamic perspective on hydrological systems offer holistic information for judging and inter-comparing soil water storage and runoff generation as well as new avenues in modeling and upscaling, which cannot be inferred from the traditional water balance thinking alone.

4 Publication of data from final reports

The DFG is entitled to publish the summary according to 3. on its websites, especially in the GEPRIS database, and to make reference to the publications listed as per 1. To be included, publications must meet the specifications set forth under 1. and credit the DFG for its financial support.

Upon request, a link to an online list of publications may be included in the database. This list of publications can be updated even after the report has been filed.

If you do not wish the summary to be published, you may request this by sending a letter or e-mail to the responsible department when you file your final report.

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