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- Improved description of small-scale processes is a key to reduce uncertainty
- Improve our understanding of hydrology through a network of observatories
- Data assimilation provides a viable approach to integrate data and models

Correspondence to:

H. Vereecken, h.vereecken@fz-juelich.de

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Soil hydrology: Recent methodological advances, challenges, and perspectives

H. Vereecken¹, J. A. Huisman¹, H. J. Hendricks Franssen¹, N. Brüggemann¹, H. R. Bogena¹, S. Kollet¹, M. Javaux^{1,2}, J. van der Kruk¹, and J. Vanderborght¹

¹Agrosphere Institute, IBG-3, Institute of Bio- and Geosciences, Forschungszentrum Jülich GmbH, Germany, ²Earth and Life Institute/Environmental Sciences, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

Abstract Technological and methodological progress is essential to improve our understanding of fundamental processes in natural and engineering sciences. In this paper, we will address the potential of new technological and methodological advancements in soil hydrology to move forward our understanding of soil water related processes across a broad range of scales. We will focus on advancements made in quantifying root water uptake processes, subsurface lateral flow, and deep drainage at the field and catchment scale, respectively. We will elaborate on the value of establishing a science-driven network of hydrological observatories to test fundamental hypotheses, to study organizational principles of soil hydrologic processes at catchment scale, and to provide data for the development and validation of models. Finally, we discuss recent developments in data assimilation methods, which provide new opportunities to better integrate observations and models and to improve predictions of the short-term evolution of hydrological processes.

1. Introduction

Water sustains life on Earth and it plays a key role in the energy and matter cycles of the terrestrial system. The status and fluxes of water in the terrestrial system are controlled by hydrological processes, which mainly take place in a thin layer of soil covering the Earth surface. Although the water content of this thin layer is only about 0.05% of the total fresh water on Earth [Shiklomanov, 1993], it plays a decisive role in controlling the major hydrological, biogeochemical, and energy exchange processes that take place at the land surface [Katul et al., 2012]. In this paper, we will focus on water-related processes that occur in the soil, and we will refer to this as soil hydrology. Soil hydrological processes are captured in the basic soil water balance equation:

$$\frac{d\theta}{dt} = P - ET - L - R - Q \tag{1}$$

where θ is the soil moisture content (*L*), *P* is precipitation (*L/T*), *ET* is actual evapotranspiration (*L/T*), *L* is drainage (*L/T*), *R* is surface runoff (*L/T*), and *Q* is lateral subsurface flow (*L/T*). This equation constitutes the basis for the description of soil hydrological processes from the point to the global scale.

The quantification and prediction of each of the terms in this equation is subject of ongoing research in the terrestrial research community including soil sciences, meteorology, hydrology, ecology, environmental engineering, and biogeosciences among others. The challenges in quantifying and predicting the terms of equation (1) have been subject of many studies, reviews, and opinions including recent publications on evapotranspiration [Wang and Dickinson, 2012], soil moisture [Robinson et al., 2008; Vereecken et al., 2014, 2013], subsurface flow [Ghasemizade and Schirmer, 2013] and runoff [McDonnell, 2013; Milliman et al., 2008; Mirus and Loague, 2013] and papers that address the full hydrological cycle [Lahoz and De Lannoy, 2014; Rast et al., 2014; Trenberth and Asrar, 2014]. In this paper, we will focus specifically on the challenges we face in the next decades to improve our understanding of the processes controlling the soil water status and the soil hydrological fluxes. We will address the potential of new technologies and modeling approaches in quantifying and predicting the key soil hydrologic fluxes in equation (1) with an emphasis on evapotranspiration, subsurface flow, and deep drainage from the field to the catchment scale. We will advocate the establishment of a network of hydrological observatories and discuss approaches to making optimal use of observations in a modeling perspective using data assimilation.

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The message of this paper is that technological and methodological advancement is a key to improving our understanding of soil hydrological processes and a prerequisite for successful testing of hypotheses. Hypothesis-driven soil hydrology needs access to high-quality data with the best possible temporal and spatial resolution to falsify hypotheses. These new technologies may also be extremely useful in improving our understanding of urban hydrology where soil hydrologic processes play an important role in e.g., ecosystem functioning of urban riparian areas, nonpoint source pollution of urban groundwater, urban brownfield wetlands, rainwater runoff, and extreme floods [*Trauth and Xanthopoulos*, 1997; *Smith et al.*, 2002; *Groffman et al.*, 2003; *Mentens et al.*, 2006; *Palta et al.*, 2014, *Schirmer et al.*, 2013]. In this paper, we will demonstrate this by presenting recent developments in technologies that have the potential to provide improved understanding of soil hydrological processes.

The importance of technological and methodological advancements for shaping our current understanding of soil hydrological processes can nicely be illustrated for the case of measuring soil moisture content across scales. In the midst of the past century, soil water status at the field scale was mainly determined by weighing and drying soil samples, using neutron probe measurements, or by installing gypsum blocks in the soil. The neutron probe measurements were labor-intensive and they required specific permission to handle the radioactive source in many countries. Gypsum blocks were simple in design, but required extensive and regular calibration and were not suited for long-term measurements. In the beginning of the 1980s, most ground-truth campaigns of remotely sensed soil moisture were still based on disturbed soil samples, which required substantial labor efforts and only provided snapshots of soil moisture dynamics.

A major breakthrough was initiated by the pioneering work of *Topp et al.* [1980] and *Topp and Davis* [1985], who developed time domain reflectometry (TDR). TDR is a measurement technique based on the propagation of high-frequency electromagnetic waves in a pair of rods that eventually allowed the acquisition of temporally highly resolved measurements of soil moisture at the laboratory, field, and catchment scale. TDR has now become a standard method in flow and transport experiments in soil columns and lysimeters, and has boosted our capacity to generate high-quality data sets of soil moisture dynamics and solute transport for the calibration and validation of soil hydrologic models. In particular, data sets became available that allowed inverse estimation of soil hydraulic and solute transport parameters in controlled laboratory experiments. In a similar manner, inverse modeling techniques allowed to estimate field-scale soil hydraulic and root water uptake parameters from TDR measurements. Nowadays, TDR measurements have developed into a reference method, and they are commonly used to validate novel soil moisture measurement techniques and solute transport data obtained from hydrogeophysical measurements [e.g., *Koestel et al.*, 2008; *Garré et al.*, 2011, 2013].

TDR measurements have also contributed tremendously to improving our understanding of the various controls on soil moisture variability at the field and catchment scale. Important findings included the identification of the presence of dry and wet states in soil moisture at the catchment scale [e.g., Western et al., 1999], the presence of temporal persistence in the vertical distribution of soil moisture in soil profiles [e.g., Pachepsky et al., 2005], the determination of convective lognormal solute transport parameters from resident concentration data [Vanderborght et al., 1996], the role of deep roots in the hydrological and carbon cycle in the Amazon [Nepstad et al., 1994], and the analysis of the decline of woody species in riparian ecosystems [Busch and Smith, 1995]. Yet, obtaining spatially highly resolved data with TDR remained challenging and expensive. New techniques, such as off-ground and on-ground ground penetrating radar (GPR) possibly embedded in a joined inversion framework [e.g., Huisman et al., 2003; Kowalsky et al., 2005; Lambot et al., 2006] and wireless soil moisture sensor networks [Rosenbaum et al., 2012; Qu et al., 2013], now provide the opportunity to obtain spatial fields of soil moisture and soil hydraulic properties. Recently, the development of cosmic ray sensors has opened the opportunity to obtain noninvasively effective soil moisture measurements for a footprint with a radius of approximately 300 m and a vertical depth of up to 70 cm [Zreda et al., 2008; Zreda et al., 2012; Desilets and Zreda, 2013; Baatz et al., 2014]. These sensors have now been placed on vehicles allowing soil moisture measurements of even large areas [Chrisman and Zreda, 2013].

The statement that technological and methodological advancements to obtain spatially and temporally highly resolved fields of hydrologic states and fluxes are critical in moving forward soil hydrological research is at a first glance conflicting with the vision paper of *McDonnell et al.* [2007], in which they conclude that despite being based on first principles and representing a high complexity, present hydrological models are

still in conflict with experimental evidence. Rather than further improving spatial description and characterization of key properties of the landscape in these models and thus reproducing process complexity, the hydrology community should explore more the underlying organizational principles that control heterogeneity and process complexity. We will argue here that both approaches need to go hand in hand. Such a combined approach was also propagated recently by *McDonnell and Beven* [2014], who pointed out the need to have access to new observation methods that will provide tools and data to evaluate models as hypotheses. We therefore expand on recent developments in modeling and data assimilation as approaches that provide a unique opportunity to improve our understanding of soil hydrologic processes and to predict soil hydrologic fluxes.

Based on these considerations, we state the need to establish a hypothesis-driven network of hydrological observatories across different climate regions interacting closely with existing networks and catchments that already measure key hydrological fluxes. This will provide an opportunity to perform distributed but coordinated field scale experiments allowing falsification of hypotheses based on high-quality data with the required spatial and temporal resolution and in combination with a long-term monitoring approach. The identification and formulation of these hypotheses are to be considered as a community effort. The establishment of such a network will improve our ability to identify underlying organizing principles that control the hydrological behavior of catchments, and will also provide a unique opportunity to answer longstanding questions in hydrology, some of which we will address in the section on establishing a network of hydrologic observatories. At present, most of the established hydrological networks and instrumented catchments were designed for practical purposes with the aim to support water management [Kirchner, 2006] rather than to verify scientific hypotheses. A network of hypothesis-driven observatories should attempt to capitalize on these existing networks and instrumented catchments and make good use of the available basic instrumentation and long-term data series.

The establishment of science-driven observational networks is common in many other science communities, such as meteorology (Fluxnet, *Baldocchi et al.* [2001]), ecology (NEON, *Hamilton et al.* [2007]), and geosciences (ICOS, *Fraser et al.* [2013]; *Peters et al.* [2014]). Fluxnet has served as a basis for many new discoveries and insights in land-surface atmosphere interactions, particularly with respect to the relationship between evapotranspiration and soil moisture [*Jung et al.*, 2010; *Williams et al.*, 2012, *Ershadi et al.*, 2014]. Testing of hypotheses requires experimental designs that are suitable to falsify or corroborate hypotheses. In many cases, such experimental designs are too expensive or the appropriate experimental equipment and techniques are not accessible to the project. This is especially the case for soil hydrological studies being performed at the field and larger scales. Such issues can only be addressed by an international effort of coordinated hydrological experiments at well-instrumented sites using state-of-the-art measurement technologies.

The remainder of the paper is organized as follows. First, we will address new methodologies that may contribute to the improved quantification of key soil hydrological processes (evapotranspiration, subsurface flow, deep drainage). We then discuss the need to establish a network of hypothesis-driven hydrological observatories in more detail. In a third section, we present and discuss approaches to better link data and models using data assimilation techniques. Finally, we present conclusions and an outlook.

2. Quantifying Soil Hydrological Processes

2.1. Disentangling the Evapotranspiration Flux

Evapotranspiration (ET) is next to precipitation the largest hydrologic flux of the terrestrial water cycle. Recent studies [e.g., Jung et al., 2010; Douville et al., 2013] based on analysis of experimental data and simulation models have shown that over the last decades the magnitude of evapotranspiration (both potential and actual) has been affected by global climate change although the sign and size of the change in ET differ strongly between regions around the globe. Jung et al. [2010] observed a significant reduction of plant water availability and land evapotranspiration in several regions of the world in the period between 1982 and 2008. They showed that global actual evapotranspiration increased on average by 7.1 mm per year per decade in the period between 1982 and 1997. Thereafter, no further increase was observed. They concluded that the cease in increase was due to soil moisture limitations in the southern hemisphere. Douville et al. [2013] reconstructed global ET between 1950 and 2005 using two land surface models (ISBA and VIC).

They showed that ET has increased in this period at mid-latitudes and that this increase is due to anthropogenic forcing. This observed increase, starting around 1980, coincides with the end of a decline in solar radiation at land surfaces observed between the 50s and 80s, so-called global dimming [Wild et al., 2005]. However, many of these ET predictions are associated with high uncertainty, mainly due to spatially and temporally variable soil water availability, with estimates ranging from 25% to 64% contribution of transpiration to ET [Wang and Dickinson, 2012], or even as high as 80%–90% [Jasechko et al., 2013]. This uncertainty is also reflected in the variability of possible functions and their parameterization that are used to partition ET in evaporation (E) and transpiration (T) [Kool et al., 2014] and to describe water uptake in macroscopic soil-plant models [e.g., Simunek and Hopmans, 2009].

The uncertainty in partitioning between T and E has important implications for predictions of water and heat exchange between the land surface and atmosphere when the duration and frequency of dry spells changes or when land-cover changes. Since plant roots can extract water from a thicker soil layer than the evaporation process, which takes place only in a thin layer at the soil surface, the time scale over which T declines during a dry spell is considerably longer than that of the evaporation process. The important role of deep roots (> 1 m) in the hydrological cycle has been recognized [e.g., Nepstad, 1994; Maeght et al., 2013] and considered in models that predict rooting depths as a function of climate and soil type [Schenk and Jackson, 2005]. Models that simulate water uptake from the root zone need to consider the interaction between spatial distributions of soil water availability and of the uptake capacity of the root system. Uptake capacity is approximated by the root length density in the most simple approach, whereas more detailed analyses use root hydraulic architectures [Couvreur et al., 2012, 2014] that are able to consider differences in root hydraulic properties between different root orders [Rewald et al., 2011]. Interaction between root uptake capacity and water availability refers to water uptake compensation (increase of water uptake from wet soil layers when part of the root zone dries out [Jarvis, 1989]) and hydraulic lift (redistribution of water in the root zone by water flow through the root system [Katul and Siqueira, 2010]). Although the relevance of water uptake compensation and root hydraulic redistribution for plant transpiration has been demonstrated [Markewitz et al., 2010; Neumann and Cardon, 2012], there is a large variability of how these processes are implemented and parameterized in terrestrial system models with consequently large variability and uncertainty in predicted T [Teuling et al., 2006].

Advances in experimental methods and designs are required to provide data that can be used to effectively reduce uncertainty about the conceptualization and parameterization of root water uptake processes. At the smallest scale, tomographic techniques that operate at the soil column scale, such as X-ray CT tomography [Carminati et al., 2009] and microtomography [Aravena et al., 2011], neutron tomography [Oswald et al., 2008; Carminati et al., 2010, Moradi et al., 2011], and nuclear magnetic resonance imaging [Pohlmeier et al., 2008, 2013], have been deployed. These studies revealed the impact of roots on rhizosphere properties (compaction and wettability) and demonstrated the effect of these properties on root water uptake. However, besides the determination of the root architecture, these methods have not been applied yet to determine root hydraulic properties. Combining these methods with models that simulate 3-D water flow in the soil and in the root system [Javaux et al., 2008, 2013] seems promising for identifying root hydraulic properties and for relating soil water distributions in soil cores to plant stress [Stingaciu et al., 2013]. After a demonstration phase of what is possible with tomographic techniques, a new phase should be started in which dedicated experiments are designed to deliver tomographic data for the validation and parameterization of soil-plant models. However, monitoring the change of water content alone may not be informative enough to obtain unequivocal flux-related root properties [Hupet et al., 2002]. The use of tracer substances may thus be of particular interest in such experiments [Zarebanadkouki et al., 2012, 2013].

Stable isotope analysis (δ^{18} O and δ^{2} H) of soil and plant water as well as T and E fluxes is a powerful tool for the identification of plant source water and the partitioning of ET fluxes in laboratory and field experiments [Wang and Yakir, 2000]. The mass differences of the major and minor water isotopologues lead to thermodynamic and kinetic isotopic fractionation effects, which thereby induce measurable differences in the isotopic composition of different terrestrial water pools (soil moisture, groundwater, surface water, plant water, and atmospheric water vapor). Since soil moisture is both essential for plant growth and the main determinant of ET, accurate measurements of soil water content and its isotopic composition at different depths are key to reliable quantification of plant water uptake as well as partitioning of ET into E and T [Nippert et al., 2010; Rothfuss et al., 2010]. Until recently, such measurements were based on destructive soil and

plant sampling followed by laborious offline analysis of the water isotopic composition in the laboratory, which allowed only for retrospective source water identification.

Recent technological advances now allow the nondestructive monitoring of stable isotope composition of soil water using gas-permeable tubing and infrared laser spectroscopy [Rothfuss et al., 2013]. It has now become possible to monitor the same soil water isotopic profile from greater depths up to immediately below the soil surface with a time resolution in the range of minutes to hours. In combination with high-frequency monitoring of the isotopic composition of the ET flux emitted from the surface and root-water uptake modeling, this approach enables to determine ET partitioning with a high time resolution. In combination with isotope-enabled SVAT models [e.g., SiSPAT-Isotope; Rothfuss et al., 2012] and root-water uptake models [e.g., R-SWMS; Javaux et al., 2008], which use these high-frequency monitoring data as input, a major advance in constraining the partitioning of ET for different ecosystems under different environmental conditions could be achieved. Field-scale applications of this combined technology are now under development. In combination with micrometeorological eddy-covariance-based isotope-specific flux measurements, this will allow field-scale analysis of ET partitioning in the near future.

First attempts are now also underway to combine isotopic characterization of water and vapor fluxes with the measurement of spatially highly resolved soil moisture profiles in the first few centimeters of the soil surface using nuclear magnetic resonance (NMR) technology. *Merz et al.* [2014] showed the potential of surface NMR to resolve the soil moisture profile subject to evaporation at the mm scale. They were able to distinguish stage 1 and 2 evaporation from bare soil based on the shape of the soil moisture profile. The shape and the profile of the soil moisture profile could only be reproduced by using a coupled model of water and vapor flow.

2.2. Quantifying Subsurface Flow and Deep Drainage

Subsurface lateral flow is widely considered to be an important hydrological flux that is poorly understood and difficult to measure and quantify. This limited ability to characterize subsurface lateral fluxes is also increasingly being recognized as a key limitation in understanding the spatial and temporal variability of biogeochemical fluxes and trace gas emissions [e.g., *Groffman et al.*, 2009; *Tang et al.*, 2014]. *Ghasemizade and Schirmer* [2013] provided a recent review of the contribution of lateral subsurface flow to the hydrological cycle. They concluded that no broad consensus exists about the mechanisms driving lateral flow processes, and that controlling factors likely depend on geology, soil properties, rainfall characteristics, and vegetation. Nevertheless, it is becoming increasingly clear that hillslope properties that are difficult to measure, such as the depth to bedrock and the presence and connectivity of preferential flow pathways, may play a key role in improving our understanding [e.g., *Freer et al.*, 2002; *Tromp-van Meerveld*, 2006a, 2006b; *Weiler and McDonnell*, 2007; *Bachmair and Weiler*, 2012]. Technological advances in our ability to measure efficiently at the hillslope scale and beyond are one possible way to gain the much needed improved understanding of subsurface lateral flow processes, and in the following we highlight advances in high-frequency isotope analysis and hydrogeophysical methods.

One possible way to distinguish different lateral flow mechanisms is by determining residence time distributions from environmental isotope tracers. Although this idea is certainly not new (see the review of *McGuire and McDonnell* [2006]), recent advances in laser-based spectroscopic methods to determine oxygen and hydrogen isotopes in water samples [e.g., *Berman et al.*, 2009; *Pangle et al.*, 2013] now allow the collection of longer isotope time series of stream water with a high temporal resolution. In the coming years, such isotope time series will become available and they are expected to test our current understanding of how water is transported and stored within a catchment [*McDonnell and Beven*, 2014].

The potential of hydrogeophysical methods to advance understanding of hydrological processes at the catchment scale has been recognized for some time now [e.g., *Robinson et al.*, 2008], but the use of this type of methods is only slowly increasing at the larger scale. However, there are a number of recent technological advances that are of great interest for soil hydrologists. For example, *Rudolph et al.* [2015] used a new generation of multireceiver electromagnetic induction (EMI) sensors measuring soil apparent electrical conductivity (ECa) for six depths of exploration to investigate the origin of observed leaf area index (LAI) patterns that indicate variable crop performance. Using EMI measurements, they found moderate to excellent spatial consistency of ECa and LAI patterns, and concluded that improved crop performance was related to a higher water storage capacity as well as subsoil clay content. Moreover, this new generation of

multireceiver EMI devices can be used to obtain quantitative information about dominant features in subsurface layering up to a depth of 2 m for areas up to several hectares in a fast and non-invasive manner [von Hebel et al., 2014]. Since bedrock is expected to provide an appropriate target for EMI because of the associated strong decrease in electrical conductivity, there is considerable potential to use EMI measurements to study how spatially variable bedrock depth beyond the m scale controls subsurface lateral flow. In addition, the potential of EMI for supporting hillslope hydrological analysis by providing a large number of distributed soil water and groundwater depth measurements with a reasonable degree of accuracy has been recognized early on [e.g., Sherlock and McDonnell, 2003]. Another technical advance is the availability of multireceiver ground penetrating radar (GPR) systems [Bradford et al., 2009], and improvements in characterizing subsurface layering can be expected from the joint application and integration of multiple geophysical methods (e.g., multireceiver GPR with multireceiver EMI).

In a push to increase understanding of lateral preferential flow, *Anderson et al.* [2009] have recently dyestained and excavated a subsurface flow network. Clearly, such excavations involve a tremendous amount of work, and noninvasive characterization of such networks would be highly preferable. Several studies have highlighted the usefulness of GPR for this task. In some settings, it is straightforward to detect soil pipes using GPR, such as in the pioneering work of *Holden et al.* [2002] in blanket peat. Recently, progress in GPR data acquisition and processing strategy has enabled a plot-scale analysis of lateral preferential flow processes [*Guo et al.*, 2014], which opens up possibilities to investigate controls on lateral preferential flow networks in a more systematic manner. The spatial resolution of such investigations could be further improved by adopting state-of-the-art 3D GPR data acquisition and processing methods [e.g., *Grasmueck et al.*, 2005; *Böniger and Tronicke*, 2010; *Kinlaw and Grasmueck*, 2012] and the use of emerging full-waveform inversion strategies for surface and crosshole GPR data [*Busch et al.*, 2014; *Klotzsche et al.*, 2013, 2014].

Although deep drainage below the root zone is important for closing the water balance in many soil hydrological settings, it seems fair to say that this hydrological flux is within the blind spot of many soil hydrologists, except perhaps those that work in semiarid and arid regions [e.g., Seyfried et al., 2005]. This is also evident from the design of many soil hydrological measurement setups, which are typically limited to the top meter of soil. Because of the general inaccessibility of the subsurface and the lack of sufficient boreholes, one of the most promising ways forward here is to rely on improved subsurface monitoring and characterization using existing and emerging hydrogeophysical measurement techniques. For example, the development of portable superconducting gravimeters now makes it possible to measure recharge fluxes in thick unsaturated zones [Kennedy et al., 2014], and the large-scale application of EMI measurements as a tool to interpolate information from scarce boreholes is also promising [e.g., Woodforth et al., 2012]. Another area of continuing progress is the integration of time-lapse geophysical measurements in hydrological models [e.g., Kowalsky et al., 2005; Lambot et al., 2006; Hinnell et al., 2010, Huisman et al., 2010; Busch et al., 2013, Leger et al., 2014], and this allows for an improved parameterization of models of the deep vadose zone to obtain more accurate estimates of deep drainage fluxes [e.g., Binley et al., 2002; Looms et al., 2008].

3. Toward a Network of Hydrological Observatories

Recent publications in the field of land surface processes demand a stronger integration of monitoring, modeling, and regionalization activities [e.g., *Katul et al.*, 2012; *Baldocchi et al.*, 2012]. The lack of such comprehensive studies hampers our ability to predict the response of terrestrial systems to changing environmental conditions (e.g., land use and climate change). Filling this gap requires a research approach that is embedded in a geographically distributed observation infrastructure. Since hydrological processes exert a fundamental control on aquatic and terrestrial metabolism and nutrient cycling, catchments represent an ideal fundamental unit of such infrastructures. For instance, more measurements on the catchment scale such as e.g., networks of eddy-covariance towers or large aperture scintillometers are needed to reduce the uncertainty range in estimating global transpiration rates [*Coenders-Gerrits et al.*, 2014]. By establishing a network of globally distributed science-driven hydrological observatories based on state-of-the-art measurement and data management technologies, hydrologic science will have a tool at its disposal to advance its science but also to better connect to the other disciplines in the Earth Science community and to address large-scale feedbacks and impacts imposed by climate change.

3.1. Existing Hydrological Observatories

In recent years, several environmental observatories have been implemented world-wide, e.g., the Critical Zone Observatory [CZO; *Anderson et al.*, 2008] and National Ecology Observatory networks [NEON, *Hamilton et al.*, 2007] in the US, the HOBE Hydrological Observatory in Denmark [*Jensen and Illangasekare*, 2011], the Heihe Hydrological Observatory in China [*Li et al.*, 2013], the Terrestrial Ecosystem Research Network (TERN) in Australia, and the Integrated Carbon Observatory Network in Europe [ICOS, *Fraser et al.*, 2013], just to name a few examples. In the following section, two national activities are presented in more detail as they are directly related to soil hydrological research.

The pilot Environmental Virtual Observatory (EVO) in the UK was a proof-of-concept project to develop new cloud-based applications for accessing, interrogating, modeling, and visualizing environmental data (http://www.nerc.ac.uk/research/funded/programmes/virtualobservatory/). National data sets, models, and uncertainty analysis approaches have been combined with cloud computing environments to explore and benchmark our current predictive capability for hydrology and biogeochemistry. The project uses catchments as integrating units to manage and visualize complex modeling results to synthesize and improve our scientific understanding and to support the management of catchments.

The Terrestrial Environmental Observatories (TERENO) initiative [Zacharias et al., 2011; Bogena et al., 2012] has been implemented in Germany. With this project, a network of integrated observation platforms has been established to investigate the consequences of global change for terrestrial ecosystems. In the framework of TERENO, long-term data series (> 15 years) of system states and fluxes will be provided to analyze and predict the consequences of climate and land use change. This comprehensive data set will be used to develop and apply integrated model systems to derive more efficient prevention, mitigation, and adaptation strategies (e.g., optimization of irrigation systems as well as development of early warning systems for extreme weather occurrences and flooding). Hydrological observatories have been implemented in which important system states and fluxes are continuously monitored (e.g., soil moisture content, (soil) temperature, and the fluxes of water, matter and energy within the continuum of the groundwater-soil-vegetationatmosphere system). The long-term data sets allow to close the local water balance [Graf et al., 2014] and to investigate the effects of land-use change (e.g., deforestation) on water, energy, and matter fluxes [Bogena et al., 2015]. High-resolution monitoring networks are also helpful for evaluating and bias correction of remote sensing measurements.

3.2. Establishing a Network of Hydrological Observatories

According to McDonnell et al. [2007], studies in experimental catchments have so far produced rather complex characterizations of catchment behavior that cannot be extrapolated or regionalized. A promising way to reduce this deficiency would be the development of systematic measurement programs that are specifically targeted to the generation of tests of new theories that allow for more concise explanations of catchment behavior. This would help to develop a catchment classification system based on dimensionless similarity indices or dominant hydrological processes [Wagener et al., 2007]. A hierarchical classification system for catchments would help to better target dominant process controls, and thus to improve predictability in the long term [McDonnell et al., 2007]. Based on nonequilibrium thermodynamics and optimality concepts, Zehe et al. [2014] proposed a classification using functional units that exhibit similar dynamics and discharge behavior. However, it is not obvious how current monitoring strategies that are mainly based on soil moisture and land surface flux observations may help in developing such classification schemes because of the non-linearity of the soil moisture redistribution processes including interactions with the land surface moisture and energy balance (open, dynamic top boundary condition), and the free, moving table (open, dynamic bottom boundary condition). Thus, it appears that observations need to be merged with models that honor the relevant nonlinear interactions in order to facilitate hypotheses testing and falsification.

The selection of sites for a global network of hydrological observatories could be based on the Budyko framework [Budyko, 1974]. This framework describes an empirical global relationship between the evaporative index and climatic dryness (or aridity) index, in which the evaporative index is defined as the ratio between actual ET and P, and the dryness (or aridity) index is defined as the ratio of potential ET to P. For instance, the Budyko framework has been used to assess the sensitivity of river discharge to climatic change [Donohue et al., 2011; Renner et al., 2012] and to analyze climate and vegetation controls on the surface

water balance and evapotranspiration [Williams et al., 2012]. The Budyko framework has also been used to describe and subdivide terrestrial systems with respect to energy-limited and water-limited systems. For instance, van der Velde et al. [2014] subdivided Sweden into three regions with unique hydroclimatic change adaptation: the mountains, the forests, and the agricultural areas. In a similar way, appropriate sites for hydrological observatories could be selected on a global scale covering a broad range of biomes and climate zones.

Hydrological observatories should be equipped with research instruments designed for long-term measurements. Important parameters, fluxes, and state variables should be monitored simultaneously to determine all components of the water and energy balance at the local scale. For instance, the turbulent exchange fluxes of energy, water vapor, and trace compounds can be monitored using eddy-covariance techniques. In addition, online stable isotope measurements of gaseous and water fluxes can provide better process understanding, e.g., separation of evaporation and transpiration fluxes [Rothfuss et al., 2012; Sutanto et al., 2012] or the assessment of transit time distributions of water and tracer compounds [Stockinger et al., 2014]. River discharge should be monitored in a nested set of subcatchments spanning distinct assemblages of hydrologic features and several orders of magnitude in drainage area. Noninvasive sensing techniques (e.g., cosmic-ray neutron probes, terrestrial gravimetry, hydrogeophysical methods) should be applied to investigate spatial and temporal variation in soil moisture content from the field to the catchment scale [Ochsner et al., 2013] because they have many important advantages over classical in-situ methods: the soil structure remains undisturbed by the measurements, the measurement device can be operated continuously (i.e., also during tilling operations), and the soil moisture measurements can integrate large areas (i.e., larger than 100 m²).

Closure of the local hydrological water and energy balances will help to understand the magnitude of measurement errors, to determine how to diagnose these errors, and to avoid misattribution of water balance components [Kampf and Burges, 2010]. For instance, Graf et al. [2014] used a 3 year long data set of eddy covariance, precipitation, runoff discharge, and spatially and temporally resolved soil moisture fields of the Wüstebach catchment to close the local water balance within 3% of the measured precipitation for the whole period.

Different measurement strategies should be considered depending on the time scale of expected changes. Rapid, short-term variations should be monitored by permanently installed instruments that have to be networked via state-of-the-art communication technology in order to enable near-real-time measurements and to simplify data management, e.g., using smart sensor networks. Smart sensor networks consist of a multitude of small sensors nodes embedded in the environment and are able to observe phenomena, e.g., temperature or soil moisture fields, with high temporal and spatial resolution. Slower variations of system states can also be observed by a system of mobile and flexible sensor networks that will operate periodically on a regular or event-driven basis thus allowing a more efficient and large-scale analysis.

A network of hydrological observatories would allow tackling a number of research questions relevant to the hydrological and soil hydrological science community and beyond: (1) What are important organizing principles that are controlling hydrological processes?, (2) Which subsurface structure-building processes are most relevant to hydrological processes?; (3) Which hydrological processes control how and when hill-slopes get connected to streams?; and (4) How important are threshold behaviors and abrupt changes occurring at timescales much smaller than the usual timescales for hydrological system dynamics?

In addition to these specific soil hydrological challenges, these observatories may contribute to addressing challenges such as the quantification of medium and long-term effects of climate and land use change on the hydrological cycle and the analysis of interface processes and feedback mechanisms between different compartments of the terrestrial system (soil, plant, atmosphere, and groundwater). The comprehensive data sets from a global network of hydrological observatories would foster the development of new modeling approaches that rely less on calibration but instead focus on an insightful analysis of landscape heterogeneity and process complexity through systematic learning from novel hydrological observation data. In addition, dedicated hydrological experiments could be accomplished in certain hydrological observatories to gain knowledge for new hydrological theories, e.g., using large-scale isotope labeling and tracer experiments. Last but not least, such a network should be complemented by interdisciplinary measuring programs that include disciplines like meteorology, geology, and ecology to embrace new scientific perspectives.

Ideally, such a network of hydrological observatories should cover the global scale, including all important climate and vegetation zones. In this way, the network could also support global modeling activities. Therefore, the network should be linked to existing global environmental programs to enable institutional support at the global scale. Examples for global environmental programs to be linked up would be UNESCOP-IHP (e.g., FRIEND), the Global Environment Facility, the Global Water Partnership, or the Global Earth Observation System of Systems (GEOSS).

4. From Observation to Prediction of Soil Hydrologic States and Fluxes Across Scales

In the previous sections, it was discussed how new technologies and observatories may allow a better characterization of soil hydrological states and fluxes. These technologies deliver spatially exhaustive data, possibly also at a high temporal resolution, that are potentially available in real-time. At the same time, terrestrial system models include more processes with a more mechanistic process description (e.g., root-soil interaction [Javaux et al., 2008]) and coupled flows of water, energy, carbon, and nitrogen between different compartments [Oleson et al., 2013]. Computational resources are ever-increasing and this type of models can now be applied at large scales with a high spatial resolution [Kollet et al., 2010].

Inverse modeling techniques aim to bring together these improved models and more and higher-quality data. Traditionally, inverse modeling in soil science focuses on estimating unknown soil hydraulic parameters, which are believed to be the most consequential ones for predicting flow and transport in the unsaturated zone. However, also unknown vegetation parameters can be included in the estimation process [e.g., *Vrugt et al.*, 2001]. Especially, Markov Chain Monte Carlo methods have become very popular for this type of parameter estimation problems [*Vrugt et al.*, 2003].

In order to represent heterogeneities, small-scale processes, and the interactions between soil, groundwater, vegetation, lower atmosphere, and streams, we need mechanistic integrated soil hydrologic models, which typically have a large number of unknown states and parameters. The model-data fusion problem for these coupled models at the catchment or larger scales include a series of specific challenges: (1) soil hydraulic and vegetation parameters are expected to vary significantly between different grid cells, (2) model predictions are affected by other important sources of uncertainty, like initial conditions (e.g., magnitude of carbon pools), soil management, and model forcings (e.g., precipitation), (3) relatively few in situ data are available at large scales and indirect information from remote sensing becomes more important as conditioning information, (4) there is a special interest for operational predictions at these larger scales (e.g., weather and flood forecasts) with the need for a real-time assimilation of measurement data, and (5) the number of unknown states and parameters is very large. Sequential data assimilation methods, and in particular the Ensemble Kalman Filter (EnKF) method [Evensen, 1994; Burgers et al., 1998] have become popular during the last 15 years in land surface hydrology because they are more suited to handle these challenges [e.g., Reichle et al., 2002]. The Gaussian assumption makes the updating step in the EnKF much more efficient and reduces the number of stochastic realizations that has to be processed to less than 1000 in most cases [Reichle et al., 2002]. The Markovian assumption further reduces the needed CPU-time [Hendricks Franssen and Kinzelbach, 2009]. In addition, EnKF (and other sequential data assimilation methods) are flexible in handling multiple sources of uncertainty and are perfectly suited for real-time data ingestion and operational predictions [Vrugt and Robinson, 2007]. Data assimilation has been used in combination with land surface models and remote sensing products to update soil moisture content in order to improve the characterization of sensible and latent heat fluxes [Lahoz and De Lannoy, 2014]. Data assimilation was historically strongly linked to the modeling of terrestrial systems at larger scales, but is recently increasingly applied as well for modeling of water flows in the unsaturated zone at smaller scales, including parameter estimation [e.g., Wu and Margulis, 2013; Erdal et al., 2014]. The Gaussian assumption made by EnKF and other DA-algorithms is more critical in such vadose zone hydrological studies because of the strongly nonlinear character of unsaturated flow. At the (small) catchment scale, sequential data assimilation has recently also been used to update the many unknown states of distributed hydrological models. Earlier work focused on data assimilation for coupled overland flow-subsurface flow models [Camporese et al., 2009; Pasetto et al., 2012]. Xie and Zhang [2010] demonstrated the potential of discharge data to update states of the distributed hydrological model SWAT. Shi et al. [2014] assimilated six different data types in a

physically based coupled subsurface-land surface model for a small 8 ha synthetic catchment that mimics the Shale Hills watershed. They show that the six unknown parameters converge toward the true values. A similar approach can be followed to assimilate various data types which are collected at the catchment scale within the context of hydrological observatories, such as campaign-based hydrogeophysical information and on-line stable isotope measurements, as discussed earlier in this paper. These new data types can be assimilated together with other more traditional data types to improve model structures and model parameterizations.

Data assimilation is especially important for integrating soil hydrological data in large-scale land-surface models. In situ data from observatories are probably more important for bias correction of remote sensing data than for direct conditioning. Concerning large-scale hydrological applications with integrated models, one could argue that although the potential of data assimilation for improving hydrological predictions of states and fluxes with land surface models was shown, benefits seem to be smaller than anticipated. It was demonstrated that remote sensing contributes to an improved characterization of upper soil moisture content both for synthetic experiments and real-world data. However, the benefit for improving estimates of root zone soil moisture content is less clear. Some studies did not find any improvement, although in many studies some limited improvement was found [e.g., Crow et al., 2008; Das et al., 2008; Barrett and Renzullo, 2009; Li et al., 2010; Draper et al., 2011]. Even for the upcoming SMAP satellite mission that will provide soil moisture information at a high spatial and temporal resolution, a preliminary synthetic study found only a small impact on improving root zone soil moisture content [Flores et al., 2012]. Recently, it was shown that the use of remotely sensed soil moisture products had a positive impact on river discharge predictions [Wanders et al., 2014]. Several reasons can be provided for the limited impact of the assimilation of remotely sensed soil moisture products for improving soil moisture characterization of the entire root zone. First, land-surface models represent subsurface water and energy cycles in a strongly simplified manner. Second, soil moisture information extracted from remote sensing is subject to different sources of errors. Third, remote sensing information on soil moisture is limited to the few upper cm of the soil. Fourth, other measured variables have been scantly used in data assimilation. Fifth, land-surface data assimilation has traditionally focused on state updating only. Sixth, data assimilation algorithms do not get the maximum information from the data due to small ensembles, poor ensembles and strong assumptions about the measurement data. We discuss these factors below, and also indicate ways forward.

Real-world studies on land-surface data assimilation used models like the Community Land Model [CLM, Oleson et al., 2013], Noah [Chen et al., 1996], or VIC [Liang et al., 1994]. All these models are based on the concept of noncommunicating columns, and neglect lateral redistribution of water and the influence of groundwater on soil moisture content. This may result in a systematic underestimation of soil moisture content in lower situated areas and an overestimation of soil moisture in elevated areas. As a consequence, systematic differences between measured soil moisture content and simulated soil moisture content can be expected, which in some cases cannot be corrected by data assimilation if the model ensemble spread is too small. A new generation of land-surface models that includes groundwater and lateral redistribution of water in a mechanistic manner is expected to achieve a better performance [Kollet and Maxwell, 2008; Brunner et al., 2012; Butts et al., 2014]. Therefore, we expect that data assimilation in combination with these next generation land-surface models will result in better predictions of soil hydrological states and fluxes.

The quality of remotely sensed soil moisture data also limits the impact of data assimilation on improving predictions of hydrologic fluxes like groundwater recharge and evapotranspiration. Remotely sensed soil moisture from passive radiometers is affected by vegetation and soil roughness. Moreover, this information is either available at a relatively high temporal resolution but coarse spatial resolution, or vice versa. In addition, a model is needed to calculate soil moisture from the measured variable (e.g., brightness temperature). These so-called radiative transfer models are also parameterized and require additional input information. At this point, we do not go further into details how each of these mentioned points can be better handled in the future, and refer to other works with more advanced discussion [e.g., Lahoz and De Lannoy, 2014]. One critical point to be stressed is that long-term observatories are important to detect biases between remotely sensed soil moisture and actual soil moisture. Bias correction is an essential component of a data assimilation system [e.g., Reichle and Koster, 2004], but the simultaneous correction of both model bias and observation bias with a data assimilation algorithm is challenging and often insufficient information is available to achieve this [e.g., Pauwels et al., 2013]. Therefore, observatories that provide data for off-line bias

correction of remotely sensed soil moisture products are very much needed. Long-term observations, which ideally cover the resolution of the remote sensing measurements, are essential for this bias correction and would increase our insight in the spatiotemporal behavior of these biases and eventually allow large-scale bias correction of remotely sensed soil moisture products. The soil moisture products with a higher resolution that are expected from the SMAP-mission will allow a better in situ verification of the remotely sensed soil moisture product.

Remotely sensed soil moisture also has a limited sampling depth, which varies from the upper few mm of soil for X-band radar to the upper 5 cm of soil for L-band radiometers. Therefore, the characterization of root zone soil moisture is often only marginally improved with remotely sensed soil moisture information. *Yang et al.* [2005] argued that soil moisture information from the top layer does not allow the identification of vertically heterogeneous soil hydraulic parameter distributions. We believe that also here additional information could give an improvement. At the field or small catchment scale, hydrogeophysical campaigns can provide this information, as argued before in this paper. Most national measurement networks of water table depth are very extensive and could provide additional information to constrain root zone soil moisture contents for large-scale applications. This is especially useful for regions with relatively shallow groundwater tables.

Most of the data assimilation studies focused on the assimilation of one observation type only (e.g., one remotely sensed soil moisture product). Multivariate data assimilation is, however, much more promising in the context of hydrological observatories, and an overview of recent work in this area is given by *Montzka et al.* [2012]. The joint assimilation of pressure head and stream discharge has been evaluated in a number of studies [e.g., *Camporese et al.*, 2009; *Bailey and Bau*, 2012]. The joint assimilation of brightness temperature (or soil moisture) and land surface temperature, which was proposed about two decades ago [*Chanzy et al.*, 1995], also received some attention [e.g., *Walker et al.*, 2002; *Barrett and Renzullo*, 2009; *Han et al.*, 2013]. However, the number of multivariate data assimilation studies is still limited, and several of them are based on synthetic data only. The assimilation of many different observation types is yet to be explored, and we see considerable potential for future research here. Long-term observatories are of special interest for such work because of the simultaneous recording of various types of variables (e.g., soil moisture, latent and sensible heat fluxes, groundwater level, leaf area index). This allows well-controlled 1-D and 3-D multivariate data assimilation experiments as a first step toward large-scale applications.

Even if the combination of improved land surface models and better soil moisture observations allows a very good reproduction of spatiotemporal variability of soil moisture content, a correct characterization of latent and sensible heat fluxes is not guaranteed [e.g., Schwinger et al., 2010; Han et al., 2014]. It is also important to calibrate effective soil hydraulic parameters, which in combination with correct soil moisture contents, are able to reproduce the land surface fluxes. Joint state-parameter estimation allows the calibration of soil hydraulic parameters, but this has hardly been applied in combination with land surface models (examples are Pauwels et al. [2009], Bateni and Entekhabi [2012] and Han et al. [2014]). Although we see the difficulty in large scale estimation of effective soil hydraulic parameters (given multiple sources of uncertainty), it is nevertheless a topic that has to be addressed. Testing and verification of joint state-parameter estimation methods is even more cumbersome than soil moisture assimilation alone, and controlled studies with data from long-term observatories are of high interest to tackle this question.

Finally, the improvement of data assimilation algorithms, and especially the ensemble generation, may also improve the characterization of subsurface and land-surface states and fluxes. Currently, little information is available for a reliable uncertainty characterization of spatiotemporal distributions of model forcings, like precipitation and short-wave and long-wave radiation. Reliable uncertainty quantification requires a definition of spatial and temporal correlations for these variables, as well as correlations among these variables. Given the importance of a reliable quantification of model uncertainty, and given the limited attention paid to uncertainty quantification of multivariate ensembles, it can be expected that a significant potential for improvement exists. Increase in computation power should allow tests with larger ensembles and give insight in the required ensemble size for successful data assimilation. Land-surface model states and observations are often non-Gaussian and are handled suboptimally by sequential data assimilation algorithms like the Ensemble Kalman Filter. Particle filters are suited for handling non-Gaussianity, but they are considered to be less appropriate for high-dimensional applications [van Leeuwen, 2009]. Although more efficient particle filters have been formulated [van Leeuwen, 2010], these have not yet been applied in hydrology. Hybrid formulations combining EnKF and particle filter also seem promising for future developments.

5. A Path Forward

Several vision and review papers have argued in the past that rather than further improving spatial description of key properties of the landscape in physics-based, spatially distributed models and thus reproducing process complexity, the hydrology community should explore more the underlying organizational principles that control heterogeneity and process complexity based on e.g., optimality and similarity theory [McDonnell et al., 2007]. This begs the question, which experimental and theoretical methodologies does the hydrological community currently have to explore these organizational principles? This question has been posed many times in the past decades [e.g., Sivapalan, 2003] but no real progress has been made up to now beyond the fact that it was recognized that a coordinated framework and theoretical formalism is needed. Both are at present still missing and the discussions are focused repetitively on the following well-known challenges.

Suggested methodologies have been and continue to be based on experiments (remote sensing and insitu measurements) and models. For experiments, even extensive measurements at the small catchment scale provide only an incomplete and uncertain picture of potential organizational principles [e.g., *Graf et al.*, 2014]. The problem is more severe for large regions and time periods, which is due to data scarcity and measurement error, and the resulting inability to capture the variability of states and fluxes at all pertinent space and time scales [*Ershadi et al.*, 2014]. For example, in case of stream discharge, absolute measurement errors are simply not known, and uncertainties may reach 25% even under engineering conditions [*Di Baldassarre and Montanari*, 2009; *Juston et al.*, 2014]. Thus, arguably, the hydrologic community will never be able to explore these principles satisfactorily with observations alone.

Regarding models, the discussion is currently focused on model complexity and hyperresolution versus model parsimony and hyperensemble simulations. The major concerns with model complexity and hyperresolution deal with the overparameterization of PDE-based models with many unknown physical parameters that are often upscaled in an ad hoc fashion [Beven and Cloke, 2012]. This may lead to nonuniqueness, and artificial confidence in simulation results, thus, also providing only limited insight in organizational principles. In turn, model parsimony generally is based on simplifying assumptions, such as perfect mixing, linearization, and also ad hoc upscaling of parameterizations resulting in e.g., linear conductance concepts and box models [Clark and Kavetski, 2010]. Kirchner [2006] pointed out that hydrological data are typically analyzed with mathematical tools that may be inherently ill suited for hydrologic systems. He refers here to the issue of "stuffing nonlinear non-additive system behavior into linear additive boxes." Applying these models in hyperensemble (inverse) frameworks may also lead to artificial confidence and uncertainty estimates. Thus, again only limited insight may be gained in organizational principles. Additionally, reactive transport simulations of biogeochemical cycles cannot be performed with such simplified models constituting a strong limitation.

In conclusion, there is no single solution to the challenge of finding organizational principles, rendering the discussion on e.g., model complexity versus parsimony largely ineffective. Instead, current methodologies for upscaling must be inventoried (including identified short-comings), which should then be incorporated in frameworks for hyperensemble data assimilation for parameter, state, and flux (uncertainty) estimation to fuse hyperresolution nonlinear modeling platforms with observations [Yuan et al., 2014]. Here we maintain that those models are useful, which allow for nonlinearity in spatiotemporal feedbacks between groundwater, soil moisture, root water uptake and transpiration by plants, evaporation from the bare ground and turbulent transfers of moisture, energy, and momentum with the atmosphere [Rahman et al., 2014]. Otherwise, the lack of degrees of freedom may result in flawed states and fluxes in the simulations, which are the result of interacting thermodynamic processes, such as precipitation and evapotranspiration at the land surface, nonlinear moisture redistribution in the vadose zone, movement of the free water table, and groundwater flow from recharge towards discharge areas. For example, in case of transient simulations including a free water table, temporal means of hydraulic pressure/head gradients do not point into the direction of the mean flux, because of the nonlinearity in the soil water retention and relative permeability relationships. Thus, temporal variability and nonlinearity needs to be resolved explicitly, since no upscaling technique is currently available to account for high-frequency variance. We also maintain that fusing so-called complex models with hyperensemble data assimilation is technically feasible in the near-future given (1) the everincreasing high-performance computing resources with exascale capabilities planned for 2020 in many computing centers around the world, and (2) the availability of open-source, massively parallel scientific

software that has been exploited only to a marginal extent in hydrology. In this path forward, monitoring across various climate regions and hydrogeologic conditions will form the basis for hypothesis testing and prognosis.

6. Conclusions and Perspectives

New technologies can greatly improve our understanding of soil hydrological processes, such as evapotranspiration, subsurface flow, and drainage. At the local scale, noninvasive techniques combined with online stable isotope analysis will help in quantifying soil water fluxes at the soil-root and the soil-plant atmosphere interfaces with high spatiotemporal resolution, whereas hydrogeophysical methods show great potential for characterizing subsurface flow and deep drainage processes at the catchment scale. We are convinced that an improved description of local-scale processes related to soil hydrological fluxes are key to reducing the large uncertainties that are still present in large-scale models used to predict these fluxes.

Hydrology, and especially soil hydrology, would strongly benefit from the establishment of a network of hypothesis-driven hydrological observatories exploiting the full potential of novel measurement technologies. Such a network would allow to better falsify hypotheses, to identify underlying organizational principles, to correct biased remote sensing data and gain increased insights in the nature of these biases and at the same time reduce the uncertainty in knowledge about states, fluxes and parameters of the hydrological system to a minimum. Linking these observations with large-scale models through data assimilation approaches offers the perspective of predicting the terrestrial water cycle at regional to continental scales.

An important but often underestimated aspect is the sustainability of research infrastructures. Although societal and scientific needs would seem to justify the long-term maintenance of hydrological observatories, researchers are typically not rewarded for ensuring viability of long-term observation systems. Furthermore, governmental financial support for the long-term operation of such infrastructures is often not secured. Therefore, finding new ways to transform hydrological observation systems from short-term research into long-term operation mode is a key challenge of the hydrological community and society.

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