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A decade of Predictions in Ungauged Basins (PUB)—a review

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A decade of Predictions in Ungauged Basins (PUB)—a review

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Abstract The Prediction in Ungauged Basins (PUB) initiative of the International Association of Hydrological Sciences (IAHS), launched in 2003 and concluded by the PUB Symposium 2012 held in Delft (23–25 October 2012), set out to shift the scientific culture of hydrology towards improved scientific understanding of hydrological processes, as well as associated uncertainties and the development of models with increasing realism and predictive power. This paper reviews the work that has been done under the six science themes of the PUB Decade and outlines the challenges ahead for the hydrological sciences community.

Key words Prediction in Ungauged Basins; PUB; IAHS; catchment hydrology; hydrological modelling; uncertainty; thresholds; organizing principles; observation techniques; process heterogeneity; regionalization

Revue d'une décennie sur les prévisions en bassins non jaugés (PUB)—une revue

Résumé L'initiative de l'Association internationale des sciences hydrologiques (AISH) sur les prévisions en bassins non jaugés (PUB), lancée en 2003 et conclue en 2012 lors du Symposium tenu à Delft (23–25 Octobre 2012), a été mise en œuvre afin de faire évoluer la culture scientifique de l'hydrologie vers une meilleure compréhension scientifique des processus hydrologiques et des incertitudes associées, et d'élaborer des modèles au réalisme et au potentiel de prévision croissants. Cet article présente une revue du travail réalisé dans le cadre des six thèmes scientifiques de la décennie PUB et souligne les défis qu'il reste à relever par la communauté scientifique hydrologique.

Mots clefs prévision en bassins non jaugés; PUB; AISH; hydrologie de bassin versant; modélisation hydrologique; incertitude; seuils; principes d'organisation; techniques d'observation; hétérogénéité des processus

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1 INTRODUCTION

At the beginning of the new Millennium, a community awareness had been reached that hydrological theories, models and empirical methods were largely inadequate for predictions in ungauged basins (PUB; Sivapalan 2003a). Furthermore, there was a need for a better comprehension of the links between the hydrological function, i.e. the way a catchment responds to input, and the form, i.e. the physical properties, of a catchment to appropriately address the challenge of ungauged basins (see Wagener *et al.* 2007, Gupta *et al.* 2008). In other words, it was realized that, in the presence of data scarcity, it would be compelling to infer hydrological function from metrics of catchment form, such as the combined effects of climate, topography, geology, soil type and land use. The vision gradually developed that such a target could only be reached by an improved understanding of the underlying hydrological processes, demanding a shift of the research focus away from parameter fitting towards process understanding and model structural diagnostics.

In addition to the quest for better prediction methods in ungauged basins, a wealth of environmental observations noted considerable change in the hydrological cycle (e.g. Costa and Foley 1999, Groisman *et al.* 2004). This has become more obvious over the PUB Decade at all scales ranging from global changes in spatio-temporal temperature and precipitation patterns (e.g. Huntington 2006, Burns *et al.* 2007, Sheffield and Wood 2008) to regional and local changes in streamflow and hydrochemical regimes (e.g. Burn and Hag Elnur 2002, Pfister *et al.* 2004, Cudennec *et al.* 2007, Didszun and Uhlenbrook 2008, Whitehead *et al.* 2009, Hu *et al.* 2011, Montanari 2012, Tshimanga and Hughes 2012). While it was recognized that these changes were most likely driven by the combined effects of a changing climate (e.g. Alcamo *et al.* 2007, Seager *et al.* 2007, Molini *et al.* 2011), land-use changes due to population or economic pressures (Verburg *et al.* 1999, Ye *et al.* 2003, DeFries *et al.* 2010) and long-term dynamics intrinsic to the hydro-climatic system (Koutsoyiannis and Montanari 2007, Koutsoyiannis *et al.* 2009), there was, at the beginning of the PUB Decade, no clear understanding of the spatial and temporal scales at which these effects would emerge (Blöschl *et al.* 2007). Together with unreliable climate projections (e.g. Koutsoyiannis *et al.* 2008a), incomplete process understanding was seen as one of the major causes of predictive uncertainty, therefore hindering meaningful predictions of the effect of change (e.g. Pomeroy *et al.* 2005).

The need to address the above challenges, especially with respect to the majority of basins worldwide that are effectively ungauged, followed from the general notion that a wide spectrum of water-related impacts was increasingly undermining the resilience of human society to water-related hazards. These issues were manifest in a range of core water areas, from flood protection (e.g. Kundzewicz and Takeuchi 1999), water supply and drought management (e.g. Vörösmarty *et al.* 2000) to water quality issues (e.g. Kundzewicz *et al.* 2008).

Despite the unique importance of water in the Earth system and hydrology's central role at the interface of numerous disciplines, prior to the advent of PUB, the discipline of hydrology remained fragmented, and lacked, for some aspects, a sufficiently strong scientific/theoretical basis to provide robust, science-based predictions (Sivapalan 2003a). The main factors contributing to the resulting predictive uncertainty, as identified by the PUB initiative, included:

(a) an incomplete understanding of the ensemble of processes underlying hydrological system response, and the catchment-scale feedbacks between these processes, frequently resulting in inherently unrealistic models with high predictive uncertainty;
(b) an incomplete understanding of the multi-scale spatio-temporal heterogeneity of processes across different landscapes and climates as the vast majority of small catchments world-wide were, and still remain, ungauged with little or no available information; and
(c) unsuitable regionalization techniques to transfer understanding of hydrological response patterns from gauged to ungauged environments due to a lack of comparative studies across catchments and a lack of understanding of the physical principles governing robust regionalization.

Thus, insufficient process understanding and the lack of concurrent data at multiple space–time scales, as well as the emphasis on localized and isolated research studies, created a situation in which reliable hydrological prediction was frequently made difficult in the relatively few gauged locations world-wide, and effectively impossible for the rest of the world.

To address these problems, the initiative for Predictions in Ungauged Basins (PUB) of the International Association of Hydrological Sciences

(IAHS) was started in 2003 with the release of a 10-year science plan (Sivapalan *et al.* 2003b). Designed as a grass-roots movement, the initiative's overarching goal was "*To formulate and implement appropriate science programmes which engage and energise the scientific community, in a co-ordinated and effective manner, towards achieving major advances in the capacity to make hydrological predictions in ungauged basins*." This strategy implied a major paradigm shift in scientific hydrology, traditionally rooted in empiricism, since it emphasized the need to move away from data- and calibration-focused methods to methods that are more strongly based on theoretical insights into physical processes and system understanding. PUB was designed to benefit the science of hydrology through providing greater coherence to the hydrological science agenda, greater coordination and harmony of scientific activities (Fig. 1), and increased prospects for scientific breakthroughs and, therefore, excitement for the science. The story of the elephant as described by blind people has since become the metaphor for the desire to move towards methods based on physical processes and system understanding.

With this overall goal, the primary research objectives of the PUB initiative were formulated:

1. to improve the ability of existing hydrological models to predict in ungauged basins with reduced uncertainty, and
2. to develop new and innovative models representing the space–time variability of hydrological processes and thereby improve the confidence in predictions in ungauged catchments.

The PUB initiative adopted several, mostly parallel, but strongly interwoven lines of research to achieve the defined objectives. The key strategy of PUB was to extract more information from data, either by more efficient exploitation of available data or by the use of newly acquired data to improve local process understanding in gauged catchments. This understanding was then to be used to design models with an increased degree of process realism at the gauged locations. At the same time, regionally or globally pooled data, together with the process knowledge from gauged locations, were to be used in comparative studies to obtain a better understanding of multi-scale, spatio-temporal heterogeneities in the patterns of hydrological response. This improved understanding of patterns was expected to facilitate the development of more sophisticated regionalization techniques necessary for extrapolating process knowledge to ungauged locations, eventually allowing more reliable predictions in ungauged basins (Fig. 2). In addition, model diagnostics were advanced to better understand uncertainties, and catchment classification methods and similarity frameworks were elaborated. This improved understanding of patterns of hydrological functioning was to provide the basis for the development of a new perspective (and its limitations), in which hydrology is not to be seen as an isolated science, but is actually the central agent at the interface of the co-evolution of climate, geology, topography and ecology and their transient and long-term responses to change. It should be noted that the focus of the PUB initiative was on predictions in ungauged basins, as well as data and process understanding to support these predictions.

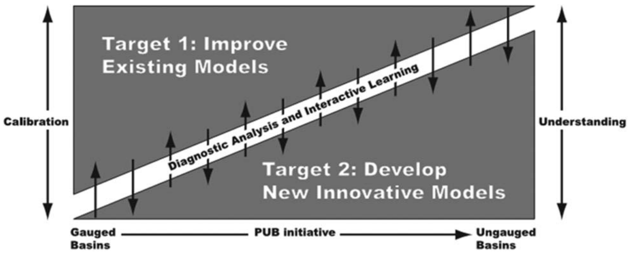
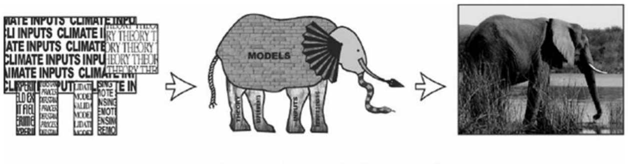


Fig. 2 In the quest for better predictions not only in ungauged basins, one initial objective of PUB was to move away from models strongly based on calibration towards those with a stronger emphasis on increased levels of understanding (from Sivapalan *et al.* 2003).

To mark the completion of the decade on Predictions in Ungauged Basins, which was celebrated with the PUB Symposium 2012, held in Delft



From a cacophony of noises to a harmonious melody

Fig. 1 The PUB initiative has been designed to lead to a greater harmony of scientific activities, and increased prospects for real scientific breakthroughs. Illustration of the elephant as described by blind people reproduced by permission of Jason Hunt (1999, from Sivapalan *et al.* 2003).

(23–25 October 2012), this paper aims to report on the many activities developed over the past decade, the major advances made and the challenges remaining in scientific hydrology. Finally, it briefly provides guidance regarding future research directions following on from the lessons learned over the past 10 years.

2 PREMISES AT THE BEGINNING OF THE PUB DECADE

In the years leading up to the beginning of the PUB Decade in the early 2000s much of scientific hydrology was driven by the quest for understanding whether physically-based, index-based or conceptual models would be preferable for reproducing hydrological processes across a wide range of catchments (see, for example, discussions in Grayson *et al.* 1992, O'Connell and Todini 1996, Beven 2001a, Todini, 2007, 2011, Refsgaard *et al.* 2010, Nalbantis *et al.* 2011). This gave rise to a plethora of models of varying complexity and developed with different underlying philosophies. These models include, but are not limited to, the *Hydrologiska Byrans Vatenbalansavdelning* model (HBV; Bergström 1976, 1992), the Variable Infiltration Capacity model (VIC; Wood *et al.* 1992), the Sacramento Soil Moisture Accounting model (SAC-SMA; Burnash 1995), GR4J (Perrin *et al.* 2003), TOPMODEL (Beven and Kirkby 1979), the Distributed Hydrology Soil Vegetation model (DHSVM; Wigmosta *et al.* 1994), the TOPKAPI model (Todini and Ciarapica 2001), and the MIKE-SHE model (Refsgaard and Storm 1995), while many more are listed and described elsewhere (e.g. Beven 2001c, Singh and Frevet 2002, Singh and Woolhiser 2002). Some of these models became more widely used than others for a variety of reasons, including, but not limited to, model simplicity, data requirements, code availability and level of documentation or dissemination of the model in the community. Some models have been used in engineering and operational hydrology practice for a long period of time and have evolved over time through the contribution of scientific testing and development. An example is the Pitman model (Pitman 1973), developed in South Africa in 1973 and in continuous use as a practical water resources assessment tool ever since, in close feedback with critical scientific scrutiny (e.g. Hughes 2004, Hughes *et al.* 2006, Kapangaziwiri *et al.* 2012). However, in spite of a considerable number of similar efforts to improve models and to meaningfully relate model structures to processes in catchments (e.g. Ambroise *et al.* 1996b, Piñol *et al.* 1997), it was not uncommon that models were applied "out of context", for situations different from those for which they had been developed. One example is the application of general hydrological land surface schemes to cold regions where many key processes were missing or highly mis-represented in the original models (Pomeroy *et al.* 1998). As a result, such models sometimes proved difficult to calibrate with parameter values difficult to explain, and frequently had limited predictive power, thereby promoting a focus on trying to get good model fits to the data, instead of trying to understand *what* was actually happening in the catchment. Unsurprisingly, this tended to hinder progress in the discipline.

During the PUB Decade, much of the progress in hydrology as a "science" was arguably owed to a handful of guiding insights that, although implicitly understood and vaguely lingering in the heads of many hydrologists long before, now became widely accepted as a necessary basis for further development in hydrology. This occurred only after a series of seminal papers explicitly addressed the relevance of these issues in a detailed manner. One of the main issues that PUB has identified was the lack of generalizable insights from the many experiments, case studies and modelling applications that hydrological research had generated. The thought-provoking discussion of Beven (2000) highlighted the varying importance of different hydrological processes, active at different time scales in different catchments, and thereby emphasized *uniqueness of place* as a consequence of the variability of nature. This led to the notion that more flexible modelling approaches could prove valuable for a better process understanding, eventually resulting in higher predictive power of models (McDonnell 2003, Pomeroy *et al.* 2007). In other words, the idea that models themselves should be systematically treated as hypotheses to be tested gained ground (e.g. Beven 2001b), and the widespread habit of implicitly postulating the validity of models was slowly abandoned, thereby opening the door for the use of models as learning tools and bringing proper use of the scientific method to bear (e.g. Popper 1959).

Similarly, several authors (Kirchner 2006, McDonnell *et al.* 2007, Wagener 2007) expanded on and strongly reiterated Klemeš' (1986) arguments that models which perform adequately well during calibration, but fail to predict the hydrological catchment response in validation, frequently do so because they do not sufficiently represent the real-world processes that control the catchment response. Rather, their often high number of parameters together with the limited number of constraints (including both calibration objectives and calibration criteria) resulted in high degrees of freedom, i.e. poorly conditioned parameter estimation problems, so that models behaved more like "mathematical marionettes" (Kirchner 2006), incapable of reproducing hydrological behaviours under conditions for which they were not previously trained (e.g. Beck and Halfon 1991, Perrin *et al.* 2001).

Critical challenges at the beginning of the PUB Decade were thus the need for more powerful diagnostic approaches and a better characterization of uncertainty estimates (e.g. Gupta *et al.* 1998). It was realized that increased physical model realism (and complexity) requires both more input data and more model parameters, which are rarely available with sufficient detail to account for catchment heterogeneity at the required resolution, meaning that some model calibration becomes effectively inevitable (Beven 2001a). In turn, the large number of calibration parameters—if they are poorly constrained by the available data—have the freedom to compensate for data error and structural weakness, and can result in considerable parameter equifinality and associated prediction uncertainty. Therefore, a widely acknowledged understanding developed that it is desirable to ensure parameters are well constrained (e.g. using orthogonal diagnostic signatures or global transfer functions to relate physical attributes to model parameters), and to ensure models have a complete and physically realistic representation of dominant processes (e.g. Franchini and Pacciani 1991). In all this work, the focus was on error propagation, i.e. how uncertainty in inputs, parameters and model structure propagates to uncertainty in runoff predictions. Increasingly, with the advent of large-sample and comparative hydrology, it was realized that there is also natural or inherent uncertainty in catchment responses, which is amenable to a more stochastic treatment than is included in the current generation of deterministic models (e.g. Koutsoyiannis *et al.* 2009). This alternative approach to uncertainty estimation has been recognized in the comparative assessment exercise carried out by Blöschl *et al.* (2013).

The need for better understanding of the connection between small-scale physics and large-scale catchment behaviour represented a further challenge. Although already suggested and discussed early on (Beven 1989a, Grayson *et al.* 1992), the importance of the fact that classic small-scale physical laws are not necessarily the sole controls of the hydrological response at the catchment scale was only starting to be fully appreciated (e.g. McDonnell *et al.* 2007). While appropriate at point, plot and, to a certain degree, also hillslope scales, their control on the hydrological response can gradually be outweighed by emerging patterns and dynamics as the spatial scale increases (see Blöschl 2001). An example is the effect of spatial covariance between catchment processes which can lead to aggregated behaviour that is very different from that expected by operation of the averaged set of processes over the catchment (Pomeroy *et al.* 2004). Very much in the sense of Aristotle, "The whole is greater than the sum of its parts", there was growing consensus that these emergent properties characterizing the ensemble of processes underlying the hydrological response are not the result of mere process aggregation, as is typically represented in bottom-up models (Beven 2000). In complex systems characterized by structured heterogeneity, such as catchments, the responses rather arise from nonlinear, yet subtle interactions and feedbacks between the processes involved, gradually manifesting themselves as scale increases (Sivapalan 2005). These considerations highlighted the limitations of aggregated performance measures, and pointed towards the use of compact signatures, constructed to describe emergent properties of the system (Eder *et al.* 2003). These signatures included, amongst others, the mean monthly variation of runoff (i.e. the regime curve), the flow duration curve, the flood frequency curve and hydrochemical variation in stream water. Top-down modelling approaches were presented that followed a systematic, hierarchical approach to the development of models of increasing complexity, guided by these runoff signatures (Jothityangkoon *et al.* 2001, Atkinson *et al.* 2002, Farmer *et al.* 2003). This constituted the functional approach to model development (Wagener *et al.* 2007).

In catchment hydrology the activation and deactivation dynamics of drainage networks, such as preferential flow paths, can be deemed such an emergent process, overriding small-scale physical laws governing flow through porous media as controlling principles (McDonnell *et al.* 2007, Spence and Hosler 2007). The development and persistence of such networks is facilitated by the co-evolution of topography, soils, vegetation and hydrology. It is therefore key to acknowledge this to better understand hydrological response patterns at the catchment scale (Cudennec *et al.* 2005, McDonnell *et al.* 2007, Savenije 2010, Wagener and Montanari 2011, Gaál *et al.* 2012). In other words, "reading the landscape" in a systems approach, as traditionally done by geomorphologists, rather than studying the physics of individual small-scale processes becomes crucial as scale increases (Sivapalan 2003a, Sivapalan *et al.* 2003b). Clearly, although landscape evolution can be described with suitable models, "reading the landscape" for hydrological purposes is still frequently a somewhat subjective *ad hoc* process of perception and, therefore, ways were sought to formalize emergent processes and to develop physically-based governing equations for describing hydrological behaviour at the catchment scale (Kirchner 2006, McDonnell *et al.* 2007). It was pointed out that, in spite of small-scale heterogeneity and process complexity, the hydrological response at the catchment scale is often characterized by surprising process simplicity (Sivapalan 2003a), which is a common feature of many complex systems (Savenije 2001, Cudennec *et al.* 2004). This led to the hypothesis that top-down models, based on catchment-integrated process representations and effective parameters (see Beven 1989a), implicitly accounting for emergent processes, are potential manifestations of system complexity expressing itself in process simplicity at larger scales (Savenije 2001), although the underlying physical theory for such top-down models was, and still remains unclear (Sivapalan 2005).

As it takes a comparative approach to learn from the differences between catchments around the world, and to shed light on catchments as complex systems, the PUB synthesis book (Blöschl *et al.* 2013) organizes the findings of the PUB Decade from the perspective of predicting runoff signatures in ungauged basins. This paper, on the other hand, reviews the achievements of the PUB Decade from the perspective of the six parallel PUB science themes—New Approaches to Data Collection, Conceptualization of Process Heterogeneity, New Approaches to Modelling, Uncertainty Analysis and Model Diagnostics, Catchment Classification and New Hydrological Theory—addressing the objectives of PUB in a constant feedback process, with local process understanding being at the interface of the six themes and serving as a common denominator.

3 WHAT HAS BEEN ACHIEVED?

3.1 Data and process heterogeneity

Data provide the backbone of any type of progress in hydrological process understanding and modelling. Both data scarcity and quality were traditionally major problems in hydrology, and are still a source of considerable uncertainty in any type of hydrological application. Sorooshian and Gupta (1983), for example, suggested that it is the quality of data, rather than the quantity, which may be the more important characteristic for a given data set (see review of observational uncertainties for hydrology in McMillan *et al.* 2012b). As traditional data acquisition is typically subject to financial, logistical and time constraints, innovations and advances in sensing technologies have the potential to be highly valuable for hydrology (e.g. Schmugge *et al.* 2002, Krajewski *et al.* 2006). During the last decade, major steps forward have been made in the availability and quality of a wide variety of environmental data obtained from different observation technologies and strategies. In addition, concerted efforts have been made in developing ways to extract more information from historical and currently already available data (see Soulsby *et al.* 2008). A critical issue is the scale-dependency of data requirements, which requires a hierarchical strategy of data acquisition, as pointed out by Blöschl *et al.* (2013). Global and low-resolution data sets, generally based on remote sensing, provide generalized information at low cost. Regional data sources of varying availability and accuracy provide more detailed information at higher cost over smaller scales. Finally, with increasing time and financial resources, local observation campaigns, even if limited to short periods, may provide a detailed understanding of the catchment response at the local scale (e.g. Blume *et al.* 2008a).

In the light of advances in data acquisition and exploitation over the last decade, there is now growing consensus that we are at the brink of an age where, in spite of reductions of many ground-based observations due to funding cut-backs, hydrology will, due to the increased availability and quality of remote sensing data, at least no longer be limited by a lack of climate data, and, where new opportunities for data assimilation are emerging, be valuable for improving predictions in ungauged basins (Troch *et al.* 2003).

3.1.1 Advances in radar and satellite technology Existing technologies, such as weather radar rainfall estimates, not only became more widely available due to an increase of areal coverage, but also uncertainties associated with the estimates could be considerably reduced (e.g. Krajewski *et al.* 2010, Moore *et al.* 2012). In addition, the different sources of uncertainty were identified more reliably, leading to an improved understanding of data quality, and enhanced methods for dealing with uncertainty (e.g.

Morin *et al.* 2003, AghaKouchak *et al.* 2009, Villarini and Krajewski 2010).

Similarly, a boost in satellite-borne observation systems gave rise to a wide variety of environmental data now readily and often freely available. For example, the NASA's Tropical Rainfall Measurement Mission (TRMM), launched in 1997, delivers 3-hourly precipitation totals over the latitude band 50° N–S at a spatial resolution of 0.25° × 0.25° (e.g. Kummerov *et al.* 1998, Huffmann *et al.* 2007). Together with suitable local calibration (e.g. Cheema and Bastiaanssen 2012), the availability of such data facilitated hydrological process and modelling studies especially in data-poor regions of Africa (e.g. Hughes *et al.* 2006, Winsemius *et al.* 2009), Asia (e.g. Shresta *et al.* 2008) and South America (e.g. Collischonn *et al.* 2008, Su *et al.* 2008); it also enabled precipitation estimation over the sea, which is crucial for the global water balance. Due to the notorious scarcity of rainfall data in these regions, this would have been difficult or even impossible otherwise. Such studies were highly instructive to better understand the link between precipitation and hydrological response patterns at regional scale. They further provided the first steps towards filling the extensive gaps in the understanding of global rainfall–runoff partitioning (e.g. Hong *et al.* 2007).

Likewise, the Gravity Recovery And Climate Experiment (GRACE), launched in 2002, provides estimates of changes in total water storage over continental areas, based on gravity anomalies at a spatial resolution of 300–400 km at monthly intervals (Rodell and Famiglietti 1999, Cazenave and Chen 2010). The possibility of independently estimating changes in water storage gave valuable insights into regional-scale storage and release dynamics (e.g. Rodell *et al.* 2007, Syed *et al.* 2008a, Hafeez *et al.* 2011), as well as into flux partitioning patterns, allowing a better understanding of the feedback between runoff, evaporative fluxes and storage change, and an improvement in the process representation in large-scale models (e.g. Ramilien *et al.* 2006, Winsemius *et al.* 2006, Syed *et al.* 2008b). GRACE has also been used for multi-objective evaluation of the performance of large-scale hydrological models in data-scarce, ungauged regions (Yirdaw *et al.* 2009).

Other missions, such as the Advanced Microwave Scanning Radiometer—EOS (AMSR-E, 25 km × 25 km, Njoku *et al.* 2003) launched in 2002 and the Soil Moisture and Ocean Salinity mission (SMOS, 50 km × 50 km, 3-day interval, Barre *et al.* 2008) launched in 2009, although still under development and thus rarely used in process or modelling studies (e.g. McCabe *et al.* 2008), show the potential to provide robust integrated estimates of soil moisture in near-surface layers (e.g. de Jeu *et al.* 2008, Cheema *et al*. 2011, Kerr *et al.* 2012). The possibility to access such soil moisture estimates will not only be essential for the improvement of the fundamental understanding of unsaturated zone processes at the catchment scale (e.g. Vereecken *et al.* 2008), but will also help to better describe the coupling of soil moisture with precipitation, evaporation and temperature at the regional scale, which will facilitate better prediction of the effects of climate change on the water cycle (see Seneviratne *et al.* 2010). Furthermore, remotely sensed soil moisture has also significant potential for improving runoff predictions in ungauged basins, as demonstrated by Parajka *et al.* (2009a) with ERS Scatterometer data.

Advances in thermal imagery technology also demonstrated its capacity to estimate soil moisture (e.g. Su *et al.* 2003). Equally important, formulations of the energy balance, based on thermal imagery, are now routinely used to obtain regional-scale evaporation estimates (e.g. Bastiaanssen *et al.* 1998, 2005, Franks and Beven 1999, Mohamed *et al.* 2004, 2006, Anderson *et al.* 2007, Senay *et al.* 2007). Further advanced remote sensing products that have proven valuable for hydrological process studies include amongst others the MODIS snow cover product (e.g. Andreadis and Lettenmaier 2006, Parajka and Blöschl 2006, 2008, Gafurov and Bárdossy 2009, Kuchment *et al.* 2010), high-resolution digital elevation models, snow depth and forest canopy characterization as obtained from airborne LiDAR sensors (e.g. Jones *et al.* 2008, Schumann *et al.* 2008, Essery *et al.* 2009, Li and Wong 2010, Hopkinson *et al.* 2012), as well as solutions to remotely sense water levels and inundated areas, providing a way to characterize spatial patterns of river discharge (e.g. Alsdorf and Lettenmaier 2003, Alsdorf *et al.* 2007, Smith and Pavelsky 2008).

The availability of such remotely sensed data allowed more effective global pooling of data (Owe and Neale 2007, Hafeez *et al.* 2011, Neale and Cosh 2012). This helped, not only in comparative approaches to identify global patterns, but also to establish tighter links between climate, catchment characteristics and hydrological function of catchments on multiple scales, thereby providing a cornerstone for deeper synthesis to identify and understand the organizational principles underlying hydrological response patterns and, eventually, for the development of a unified hydrological theory.

3.1.2 Advances in ground-based observation technology During the PUB Decade, advances in quality, availability and accessibility of remotely sensed data were, albeit with limited reduction of uncertainty, complemented by considerable innovations in ground-based observation technology, including new methods for streamflow measurement (e.g. Hilgersom and Luxemburg 2012, Tauro *et al.* 2012), microwave links for estimation of precipitation and evaporation (e.g. Leijnse *et al.* 2007a, 2007b), or wireless technologies for data transmission (e.g. Bogena *et al.* 2007, Trubilowicz *et al.* 2009). Further examples include the exploration of geophysical methods, whose potential for hydrological applications, especially for hillslope-scale soil moisture estimation (Robinson *et al.* 2008), has only now begun to be acknowledged. While the methods and protocols for ground-penetrating radar soil moisture estimation are comparatively well developed (e.g. Huisman *et al.* 2003, Lunt *et al.* 2005), the utility of electrical resistivity surveys for soil moisture estimation (e.g. Samouëlian *et al.* 2005) is still limited due to calibration difficulties and redundancies in interpretation. However, its potential in combination with other field methods (e.g. tracer methods) has been demonstrated (e.g. Uhlenbrook *et al.* 2008).

In contrast to large-scale, satellite-based gravity observations (GRACE), terrestrial gravity measurements proved to be valuable, not only to assess soil and aquifer properties (e.g. Jacob *et al.* 2008), as well as water storage dynamics on event and small catchment scales (Creutzfeld *et al.* 2012), but also to evaluate hydrological models (e.g. Naujoks *et al.* 2010). Some studies explored and highlighted the value of ground-based thermal imagery for flow paths and in-stream process identification on the plot/hillslope and reach scales. While Deitchman and Loheide (2009) demonstrated how thermal imagery can be used to visualize saturated–unsaturated zone transitions at a groundwater seepage face, Cardenas *et al.* (2008) used a thermal camera to describe detailed in-stream temperature dynamics. Others showed how thermal imagery can be used to trace riparian water sources to better understand hillslope–riparian–stream connectivity (Pfister *et al.* 2010), and to detect and quantify localized groundwater inflow into streams (Schuetz and Weiler 2011), both of which are crucial for more in-depth understanding of the thresholds and dynamics of multiple interacting flow paths through which water is routed at the hillslope scale. In a different application, Pomeroy *et al.* (2009) showed how ground-based thermal imagery can be used to improve the conceptualization of forest canopy energetics algorithms in snowmelt models. Similarly, based on image processing technology, Floyd and Weiler (2008) and DeBeer and Pomeroy (2009) demonstrated the utility of off-the-shelf digital cameras for measuring snow accumulation and ablation dynamics. In addition, a portable snow acoustic reflectometry gauge has provided a non-destructive technique to measure snow water equivalent from ground surveys (Kinar and Pomeroy 2009).

The development of distributed temperature sensing (DTS) techniques using fibre-optic cables (e.g. Selker *et al.* 2006b) resulted in a variety of potential applications, helping to characterize and conceptualize a range of hydrological processes, from stream temperature dynamics (Westhoff *et al.* 2007), snow thermal processes (Tyler *et al.* 2008) and soil moisture estimation (Steele-Dunne *et al.* 2010) to hyporheic exchange (e.g. Slater *et al.* 2010, Westhoff *et al.* 2011, Krause *et al.* 2012) and urban-hydrological applications in sewers (Hoes *et al.* 2009). An example of the DTS technique is shown in Fig. 3, which illustrates the potential of spatial and temporal high-resolution observations that may reveal patterns and processes otherwise undiscovered. During the day time the stream water is warmer than groundwater, so the subsurface inflow sources into the stream are indicated by sudden decreases of the stream temperature along the stream course. Conversely, during the night or early in the morning the stream water is colder than groundwater, so there are sudden increases in the temperature. Based on these observations and a number of assumptions on the thermal characteristics of the system, the exchange fluxes can be estimated.

During the PUB Decade, developments outside of hydrology, such as the rise of the open source Arduino development board (arduino.cc/en), allowed hydrologists to develop their own electronic sensors more easily. The range of hydrological measurements was extended by using off-the-shelf sensors, such as accelerometers to measure precipitation (Stewart *et al.* 2012), or game-console remotes to measure water levels (Hut *et al.* 2010), and also measuring tree canopy interception by monitoring stem compression (Friesen *et al.* 2008).

In contrast to remotely sensed information, ground-based observation technology contributed to deepen the detailed process understanding at the local scale. On the way towards the development of a unified hydrological theory, these data will be instrumental for comparative studies to link larger-scale patterns and climatic influences to local hydrological

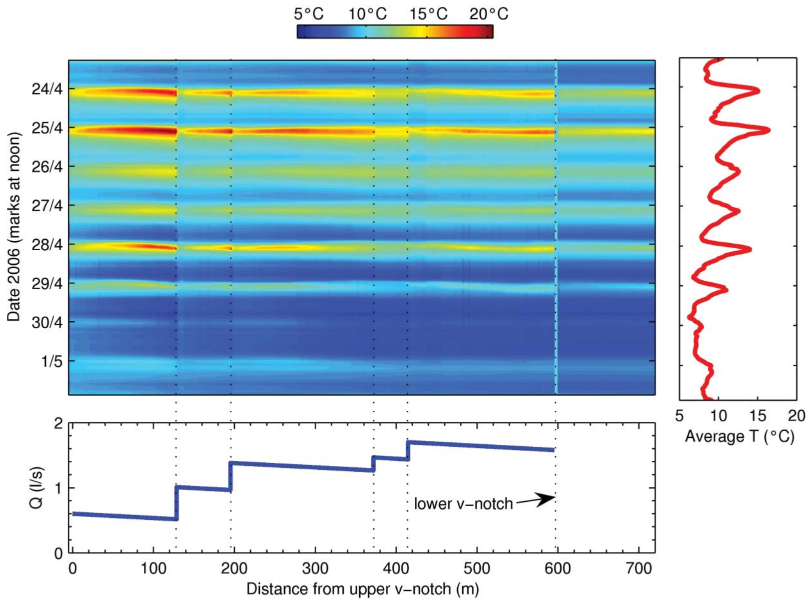


Fig. 3 Observed continuous longitudinal and temporal temperature profile of the Maisbich stream in Luxembourg between 24 April and 1 May 2006. Clear temperature jumps can be seen at the location of the groundwater inflows (from Selker *et al.* 2006a, © 2006 John Wiley and Sons).

function of catchments. Note that, for brevity, only some highlights of advances in observational technology are given here and many more observation methods were and are currently being developed.

3.1.3 New data and advances in process understanding through experimental studies

New data became available, not only through new technologies and higher observation resolutions, but also—and maybe even more importantly for the fundamental understanding of the link between hillslope- and catchment-scale hydrological processes—through a vast number of in-depth experimental studies. These studies focused on individual or specific aspects of the system and often provided crucial insights into catchment internal water flow dynamics, helping to shape our perception of how water moves through a catchment.

Many of these studies involved detailed observation of variables, such as runoff in nested subcatchments, piezometric levels, soil moisture or tracer dynamics, all of which are sometimes collectively referred to as “orthogonal information” (e.g. Winsemius *et al.* 2006, Fenicia *et al.* 2008c), a term that can be misleading, as clearly not all of the variables are strictly independent of each other. The availability of these data in a number of research catchments led, for example, to the insight that in many catchments the groundwater dynamics in the hillslope and riparian zones are effectively decoupled, implying fundamentally different process dynamics for these different landscape elements (e.g. Detty and McGuire 2010). For example, McGlynn and McDonnell (2003) and McGlynn *et al.* (2004) found in the Maimai catchment in New Zealand that, with increasing catchment wetness, runoff generation shifts from the riparian zone to the hillslope, which is largely corroborated by the results from other hillslopes and catchments in different climates and landscapes (e.g. Seibert *et al.* 2003b, Stieglitz *et al.* 2003, Molénat *et al.* 2005, Uchida *et al.* 2006, Jencso *et al.* 2009, Anderson *et al.* 2010). As emphasized by Seibert *et al.* (2003b), the generality of the steady-state assumption, i.e. groundwater levels rise and fall uniformly over the hillslope and in phase with runoff, as for example implemented in the original version of TOPMODEL (Beven and Kirkby 1979), thus needed to be rejected in favour of more flexible conceptualizations now routinely incorporated in rainfall–runoff models (e.g. Beven and Freer 2001a, Seibert *et al.* 2003a, Birkel *et al.* 2010a).

Tightly linked to transient groundwater dynamics are the pattern and dynamics of stormflow generation as already described, for example, by Hewlett and Hibbert (1963), or Whipkey (1965). Although the potential importance of preferential flow as a potential stormflow generation process was realized early on (e.g. Hursh 1944, Jones 1971, Beven and Germann 1982, McDonnell 1990, Montgomery and Dietrich 1995, Sidle *et al.* 1995), the heterogeneity of preferential flow paths and the lack of suitable observation techniques made its influence on runoff generation difficult to understand. Only recently, a number of process studies, based on a mix of the orthogonal data outlined above, elucidated the role of preferential flows in runoff generation and brought the concept closer to mainstream hydrology. Besides getting a better understanding of the spatio-temporal distribution of preferential flow structures and the resulting implications (e.g. Sidle *et al.* 2001, Vogel *et al.* 2005, Zehe *et al.* 2007), some studies emphasized the importance of preferential infiltration and recharge (e.g. Zehe and Flühler 2001, Weiler and Flühler 2004, Blume *et al.* 2008b, Salve *et al.* 2012), especially under dry conditions, as envisaged earlier by Horton (1940, see also Beven 2004). Exploring water exchange processes between the soil matrix and macro-pores, Weiler and Naef (2003) also found evidence that preferential flow paths can rapidly activate subsurface stormflow as water effectively bypasses the soil matrix, a conclusion that was later supported by the results of similar studies (e.g. van Schaik *et al.* 2008, Anderson *et al.* 2009, Legout *et al.* 2009). In other studies, the temporal dynamics of the generally threshold-driven preferential flow were explored and found to be mainly controlled by antecedent wetness (e.g. Buttle and McDonald 2002, Uchida *et al.* 2005b).

A further stormflow generation mechanism, complementary to preferential flow, first suggested by Hewlett (1961), was further elaborated on by Spence and Woo (2003, 2006), also reflecting the results of McNamara *et al.* (2005), who argued that, in order to generate runoff, water moving through the soil towards the stream needs to first satisfy soil moisture deficits along its flow path. In other words, soil needs to “fill” up to a certain threshold before it can “spill”: the “fill-and-spill” hypothesis. This concept was extended by Tromp-van Meerveld and McDonnell (2006b) with data from an experimental study at the Panola hillslope (Tromp-van Meerveld and McDonnell 2006a). They also demonstrated that a certain precipitation threshold needed to be exceeded in order to generate runoff. However, they explicitly linked the fill-and-spill mechanism to irregular bedrock topography (see Freer *et al.* 2002). They argued that the build-up of transient groundwater on the soil–bedrock interface of a hillslope does not immediately generate local lateral flow, but must first fill depressions in the bedrock topography along the flow route before the entire hillslope is sufficiently connected to generate runoff. The fill-and-spill mechanism has been used to describe the variation of catchment contributing areas to stormflow in poorly drained landscapes with substantial depression storage that result from Pleistocene glaciation, such as bed-rock lake and wetland dominated drainage systems (Spence *et al.* 2010, Phillips *et al.* 2011), or prairie wetland dominated systems (Shook and Pomeroy 2011). An implication of fill-and-spill mechanisms can be the potential absence of a unique relationship between storage and runoff efficiency in some of these catchments, and that runoff response can display threshold behaviour depending on the catchment “memory” of connectivity in flow systems (e.g. Moore 1997, Spence 2007), and so the catchment-scale connectivity of surface depression storage must be considered in order to estimate the hydrological response to inputs of rainfall or snowmelt.

Irrespective of the underlying processes, several studies investigated actual stormflow generation thresholds and what is controlling them on the hillslope and small catchment scales. Although flood characteristics are generally highly site specific, a common baseline from process studies, supporting earlier assumptions, was shown to be that stormflow generation and event runoff coefficients are controlled, not only by event precipitation volumes, and antecedent wetness (e.g. Meyles *et al.* 2003, Merz *et al.* 2006, Detty and McGuire 2010, McGuire and McDonnell 2010, Penna *et al.* 2011), but also by event precipitation intensity (Blume *et al.* 2007, Hrachowitz *et al.* 2011b), stream network connectivity (Jencso *et al.* 2009, Jencso and McGlynn 2011, Phillips *et al.* 2011) and storm and inter-storm duration (Carrillo *et al.* 2011).

However, it is important to note that the thresholds that must be exceeded to activate flow on the small scale, e.g. to activate *one* soil pipe, are very different from thresholds triggering flow on the hillslope or at the catchment scale (Hopp and McDonnell 2009, Michaelides and Chappell 2009, Zehe and Sivapalan 2009). An increasing understanding thus developed that hillslope or catchment *response thresholds* are reflections of the amount of water needed to activate a sufficient number of intermittent small-scale processes, each characterized by an individual *process threshold*, and to establish hydrological connectivity over the entire domain (Fig. 4, Troch *et al.* 2009a, Zehe and Sivapalan 2009, McMillan 2012, Ali *et al.* 2013). The difference between these thresholds is tightly linked to the predictability of the system. As thresholds introduce switches in the regime, uncertainties in the initial conditions can result in

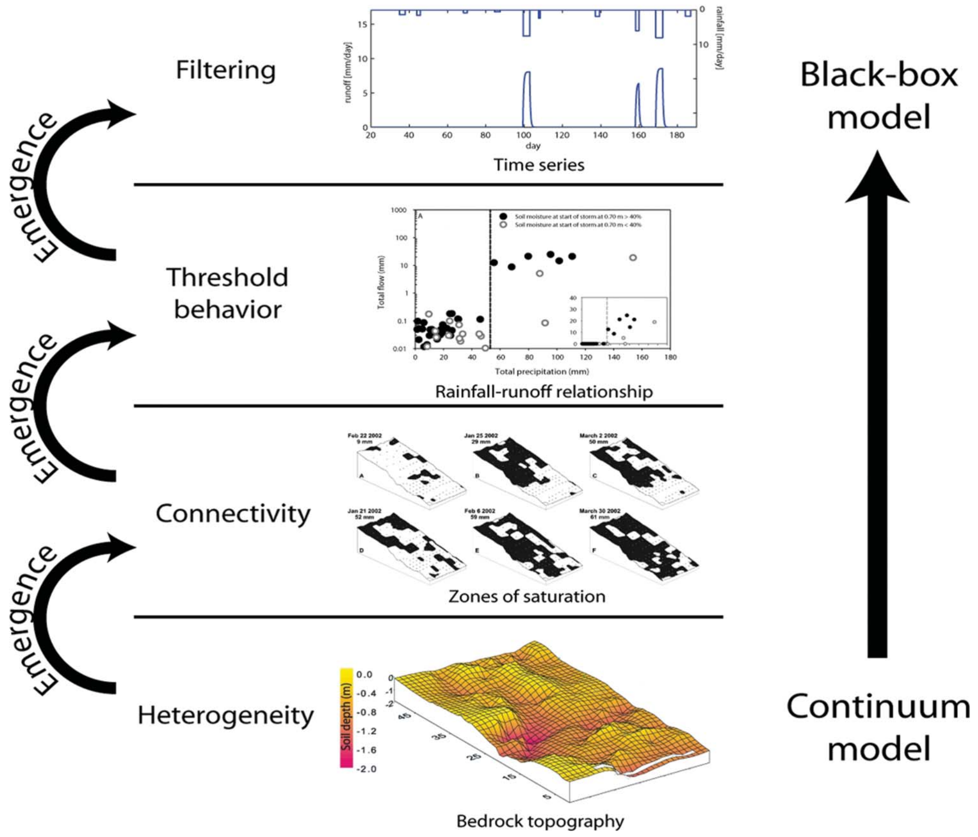


Fig. 4 Based on earlier work by Tromp-van Meerveld and McDonnell (2006a, 2006b), this figure illustrates how local heterogeneities in the subsurface, such as soil pipes, control the hillslope connectivity, and as emergent properties in turn give rise to threshold-like subsurface stormflow response on the small catchment scale (from Troch *et al*. 2009a, with permission Ciaran Harman, © 2008 Blackwell Publishing Ltd.). It indicates the importance of distinct thresholds controlling emergent behaviour at different scales from the plot to the catchement scale.

considerable prediction errors. This results from the fact that small differences in available water determine whether the system reaches the tipping point, or the response threshold, at which it switches quasi-instantaneously from one regime to another, as shown by Zehe and Blöschl (2004). Thus the smaller the scale of interest and the closer the state of the system is to a certain threshold, the poorer the predictability (Blöschl and Zehe 2005). The threshold effects discussed above are supported by, for example, the results of hillslope experiments by Anderson *et al.* (2009), who found that flow velocities in preferential flow features were higher when measured over shorter rather than longer distances as "*flow paths are more likely to be connected over shorter than longer distances*." Similarly, Jencso *et al.* (2009) showed that hillslope–riparian–stream water table connectivity can be a function of contributing area, where large contributing areas cause continuous connection, while small ones lead to transient connections. This also reflects the results of Western *et al.* (2001), who found that connectivity may change during the year in response to the seasonal cycle of soil moisture. In a modelling study using percolation theory, Lehmann *et al.* (2007) were able to reproduce the considerably nonlinear response of the Panola hillslope using randomly distributed soil properties, thereby lending further support to the importance of threshold-based connectivity. A detailed overview of the concept of hydrological connectivity is given by Bracken and Croke (2007).

Although understanding runoff generation and the mechanisms of water release in catchments is a central question in hydrology, an increasing number of studies also highlighted the need for improving our understanding of how catchments retain water (McNamara *et al.* 2011). This is essential, since: "*Changes in storage moderate the fluxes and exert critical controls on a wide range of hydrologic, chemical and biologic functions of a catchment*" (Tetzlaff *et al.* 2011b). For example, in detailed studies (Spence 2007, Spence *et al.* 2010, Phillips *et al.* 2011), it was found that the spatial distribution of headwater storage is critical for determining which parts of a catchment contribute to runoff. These studies showed further that the efficiency of a catchment to generate runoff from precipitation depends on where water is stored and on how accessible the storage is to the outlet. Based on detailed field mapping of surface runoff generation types and hydrogeological storage, Rogger *et al.* (2012a, 2012b) have shown that catchment storage can indeed lead to threshold behaviour similar to macropores.

A wide range of process studies was also dedicated to cold-region hydrology (see Carey and Pomeroy 2009), with an emphasis on understanding the feedback processes constituting atmosphere–surface energy exchange and thus the accumulation–ablation dynamics of snow (e.g. Pomeroy *et al.* 2003, Granger *et al.* 2006), including the relevance of wind redistribution of snow, and sublimation (MacDonald *et al.* 2010), but also addressing spatial variability of snow-related processes (Pomeroy *et al.* 2004, Clark *et al.* 2011c), the importance of vegetation on snow-pack dynamics (Pomeroy *et al.* 2006, Jost *et al.* 2007, Ellis *et al.* 2011), and the importance of these processes in controlling the contributing area for runoff over frozen ground (DeBeer and Pomeroy 2010) and streamflow generation (Quinton and Carey 2008, 2009, Fang *et al.* 2010, Pomeroy *et al.* 2012).

The wealth of data from process studies during the PUB Decade was instrumental in raising the hydrological community's awareness of the relevance of thresholds and the potential of complex interactions between threshold-controlled processes (Ali *et al.* 2013), which is critical for avoiding misinterpretations of the frequently simple response patterns of systems of organized complexity, such as catchments. This is true in particular for threshold-controlled network dynamics for flow generation. However, in spite of considerable advances in detailed process understanding, a wide range of questions still remains to be answered, such as whether a general theory of preferential flow can be formulated as a self-organizing system (e.g. Beven 2010). In the adoption of comparative approaches for synthesis, data acquired from process studies are valuable to establish stronger links between the hydrological function of individual catchments, their physical properties and climate. This will be a critical step towards identification of organizational principles and the formulation of a unified hydrological theory (Sivapalan 2005). A potentially important component of this endeavour may be the use of controlled experimentation (e.g. Rodhe *et al.* 1996, Kendall *et al.* 2001, Holländer *et al.* 2009). Kleinhans *et al.* (2010) argued that many major issues in hydrology are open to controlled experimentation. We will address this issue further in Section 4.

3.1.4 Tracer data and advances in the understanding of transport processes Data obtained from tracer and nutrient transport studies were also highly instructive in advancing the understanding of transport processes and to better link them to the hydrological response. On the hillslope scale, these data helped to improve the conceptualization of mixing processes in the soil. In contrast to common modelling assumptions, complete mixing was realized to be too simplistic to explain transport processes of solutes and particles mainly due to bypass flows in macropores as well as plant transpiration (e.g. Weiler and Naef 2003, Grimaldi *et al.* 2009, Brooks *et al.* 2010, Königer *et al.* 2010, Rouxel *et al.* 2011, Klaus *et al.* 2013). At the catchment scale, tracer data helped to understand why stream chemistry frequently exhibits dynamics that are deceptively inconsistent with the runoff response (see Zuber 1986, Kirchner 2003), which was reflected in the prolonged debate on why stormflow mostly consists of "old" water (e.g. Pinder and Jones 1969, Sklash and Farvolden 1979, Beven 1989b, McDonnell 1990, Bishop 1991). In most catchments, water is released as discharge over various flow paths. Some of these flow paths, such as macropores, transport water and tracer particles to the stream according to an elevation head in an advective process, which can result in relatively small time lags between the runoff and tracer responses, while other flow paths, such as groundwater, rather translate pressure waves according to a pressure head, sometimes referred to as diffusive processes (Berne *et al.* 2005, Harman and Sivapalan 2009). The translation of pressure waves, however, entails an effective decoupling of the hydraulic and tracer responses, i.e. a phase shift, as the celerity of the pressure wave is different from the particle flow velocities (Beven 1989b, 2001c, Weiler and McDonnell 2007, McDonnell *et al.* 2010).

Correspondingly, the general pattern of transport processes, and thus the sensitivity of catchments to contamination, were in many catchments—mostly based on steady-state analysis—also found to be controlled by the permeability and storage capacity of both soils and bedrock (e.g. Soulsby *et al.* 2004, 2006a, Dunn *et al.* 2007, Tetzlaff *et al.* 2007b, Sayama and McDonnell 2009, 2009a, Katsuyama *et al.* 2010, Speed *et al.* 2010, Harman *et al.* 2011, McGrane *et al.*

2013), whereas in other regions, flow-path lengths (or drainage density) and gradients, or a combination of these factors, emerged as more significant descriptors (e.g. Arheimer and Brandt 1998, McGuire *et al.* 2005, Hrachowitz *et al.* 2009a, Tetzlaff *et al.* 2009b, Lyon *et al.* 2010a). Flow into and over thawing frozen ground can dynamically alter flow paths and hydrochemical dynamics, and so frozen soil thermodynamics must be considered in understanding flow paths in cold-region catchments (Lilbaek and Pomeroy 2007, 2008). In addition, tracer data have allowed assessment of the temporal dynamics of transport processes and, consequently, the assumption that water transit times are wetness dependent became a well-established hypothesis (e.g. McGuire *et al.* 2007, Roa-Garcia and Weiler 2010, Botter *et al.* 2011, Rinaldo *et al.* 2011, Hrachowitz *et al.* 2013). Further studies analysing the temporal dynamics in response patterns of transport processes identified antecedent moisture conditions, event precipitation and evaporation as first-order controls on the shape of transport process response functions (e.g. Hrachowitz *et al.* 2009b, 2010b, Van der Velde *et al.* 2010, Harman *et al.* 2011, Heidbüchel *et al.* 2012, McMillan *et al.* 2012a). However, Hrachowitz *et al.* (2013) pointed out that, to explain the frequently observed hysteresis effects in discharge–tracer concentration relationships (e.g. Weiler and McDonnell 2006), it is necessary to take into account not only the amount of water stored, but also where and how in the system it is stored, as previously also highlighted by others (e.g. Moore 1997, Spence and Woo 2006).

In addition to the continued use of non-conservative tracers, such as water temperature (e.g. Moore *et al.* 2005a, 2005b, Gomi *et al.* 2006), the increasing availability of a new generation of tracers, including smart tracers, such as Resazurin (Haggerty *et al.* 2008), synthetic DNA (e.g. Ptak *et al.* 2004, Foppen *et al.* 2011), bacteria (Lutterodt *et al.* 2012), diatoms (Pfister *et al.* 2009) and RFID antennas (Schneider *et al.* 2010), will prove highly beneficial. Such technologies are expected to advance the understanding of catchment-scale transport, especially with respect to enhancing the understanding of mixing processes in different parts of the system (e.g. Legout *et al.* 2007, Van Schaik *et al.* 2008, Godsey *et al.* 2009, Stumpp and Maloszewski 2010, Van der Velde *et al.* 2012, Hrachowitz *et al.* 2013, Klaus *et al.* 2013), which is critical for assessing the ability of catchments to moderate water fluxes, their response and sensitivity to contamination, e.g. peak contamination loads or the persistence of contamination, as well as their resilience to climate and land-use change, thereby providing information on the way individual catchments function.

3.1.5 Advances in understanding of scale dependence through increased data coverage and resolution Hydrological processes exhibit remarkable heterogeneity at all spatial and temporal scales. In spite of an increased conceptual and quantitative understanding of scaling properties in natural systems (e.g. Gupta *et al.* 1986, Blöschl and Sivapalan 1995, Rodríguez-Iturbe and Rinaldo 1997) and their application in models, such as the geomorphological instantaneous unit hydrograph concept (GIUH; Rodriguez-Iturbe and Valdes 1979), the question of how these scaling properties actually link to process heterogeneities across different scales (see Dooge 1986) remained largely unexplored at the beginning of the PUB Decade. Yet, it was recognized that better insights into scaling relationships are the key to identifying the overarching process controls and eventually to the development of a unified hydrological theory (Sivapalan 2005). Observing hydrological processes at multiple scales and characterizing their variability should thus be followed by interpretation in terms of underlying heterogeneities in order to identify the overarching process controls (Sivapalan 2005). It is of interest to investigate not only the scale-dependence of processes, but also the presence of thresholds below which process integration dominates over the emergence of new processes.

Many of the aforementioned advances in observation technology allow higher spatial and temporal coverage and resolution of data, critical for hydrology, as the scale at which many environmental variables are observed determines which and how much of the system's patterns and dynamics become visible to us (see Kirchner *et al.* 2004). It was realized that, due to the nonlinearity of the hydrological system, the need for spatial and temporal averaging or inter-/extrapolation, as determined by the observation scale, can generate considerable bias in both process conceptualizations and model results (Andréassian *et al.* 2004b, Bárdossy and Das 2008, Das *et al.* 2008, Dornes *et al.* 2008a, Fenicia *et al.* 2008b, Jost *et al.* 2009, Kumar *et al.* 2010, Kavetski *et al.* 2011, Singh *et al.* 2012).

For example, a study by Olden and Poff (2003) revealed changing correlations between daily, monthly and annual hydrological indices, which can be observed in different spatial similarity patterns for different catchment-scale signatures (Sawicz *et al.* 2011), thus indicating the different information content of different temporal scales as underlined by Wagener *et al.* (2007). Similarly, it can be demonstrated that landscape and climate controls on hydrological response pattern are a function of the temporal scale (Son and Sivapalan 2007). However, the lack of suitable observation techniques dictates the need for temporal averaging in many applications (e.g. precipitation sampling for chemical analysis), thereby reducing peaks, introducing phase shifts, and potentially concealing system-relevant response patterns and processes featuring shorter time scales (e.g. Bronstert and Bárdossy 2003, Hrachowitz *et al.* 2011a). While basic hydro-climatic variables, such as precipitation, temperature and stream stage, are routinely available at relatively high temporal resolutions, frequently with observation intervals of 1 h or less, especially the long-term, high-frequency retrieval of water samples for chemical analysis is still difficult. However, a handful of projects, sampling precipitation and stream water at sub-daily and daily intervals, showed the value of such data for learning more about the short-term dynamics of stream water chemistry and catchment-scale transport processes (Kirchner *et al.* 2000, Tetzlaff *et al.* 2007a, Berman *et al.* 2009, Birkel *et al.* 2012, Neal *et al.* 2012).

Complementary to efforts on the plot and hillslope scales (see Section 3.1.3), a variety of studies also attempted to explore the potential emergence of different processes, i.e. spatial scale dependency and threshold behaviour, on the catchment scale. While some studies found evidence for relationships between catchment processes and catchment scale (e.g. Wolock *et al.* 1997, Buffam *et al.* 2007, Buttle and Eimers 2009, Dawson *et al.* 2009, Frisbee *et al.* 2011, Tetzlaff *et al.* 2011a), results of other studies tend to support process convergence at the scale of the study catchments; in other words, they support the notion that downstream response patterns reflect the integrated or averaged upstream influences without further unaccounted processes emerging (e.g. McGlynn *et al.* 2003, Shaman *et al.* 2004, McGuire *et al.* 2005, Uchida *et al.* 2005a, Soulsby *et al.* 2006b, Asano *et al.* 2009, Tetzlaff *et al.* 2009b, Capell *et al.* 2011), thereby highlighting the importance of headwaters (see Bishop *et al.* 2008). Interpreting these findings, Frisbee *et al.* (2012) argued that, on the catchment scale, there is evidence that the presence and degree of scale dependence are a manifestation of the degree of spatio-temporal process heterogeneity in catchments. Thus, when a scale is reached that is larger than the scale of the underlying process, scale dependence is lost (e.g. Asano *et al.* 2002, Shaman *et al.* 2004, Hrachowitz *et al.* 2010a), which, however, in the case of multifractal variability (e.g. precipitation), or at larger scales of variability, might never be the case. However, in spite of considerable progress in the understanding of spatial scale dependence, aspects of the question, in particular those related to predictability, still remain unresolved (see Ali *et al.* 2013).

3.2 Models, uncertainty analysis and diagnostics

3.2.1 Advances in model structure design and modelling strategies Until the beginning of the PUB Decade, the proliferation of off-the-shelf modelling software led to a polarization between different *modelling* groups and substantial effort went into determining what model types (physically-based models *vs* index models *vs* conceptual models) were *universally* preferable. There was a tendency to hide behind acronyms, which blocked the communication and the advancement of science. In other words, instead of testing the most suitable model for a particular “unique” catchment setting, which is also often constrained by a lack of suitable data, leaving all tested model designs equally uncertain (Hughes 2006, Uhlenbrook *et al.* 2010), a model code was often examined for its ability to be universally applicable. The universal use of the same code has a number of advantages, such as limited requirement for training of personnel (Le Moine *et al.* 2007), better understanding of parameter dependencies and easier regionalization (Oudin *et al.* 2008a), and a number of models have indeed been demonstrated to be applicable across a wide range of climate and physiographic conditions (e.g. Hughes 1997, Perrin *et al.* 2003, Gan and Burges 2006, Pietroniro *et al.* 2007, Semenova and Vinogradova 2009, Carrillo *et al.* 2011, Vinogradov *et al.* 2011, Strömqvist *et al.* 2012).

During the PUB Decade, an increasing understanding of the importance of openness towards different approaches, and the willingness to communicate and search for opportunities developed. In other words, modelling started to be more curiosity- and less prestige-driven than before. This led to a much more open attitude towards modelling and cross-fertilization between concepts, for example mixing mechanistic descriptions with data assimilation, experimenting with algorithms, merging methods and using multi-basin approaches to test assumptions, agreeing that no model is perfect. The modelling process and assumptions involved became more important than the model acronym. Several model comparison studies (e.g. Gan and Burges 1990b, Francini and Pacciani 1991, Perrin *et al.* 2001, Reed *et al.* 2004, Duan *et al.* 2006, Rutter *et al.* 2009) supported this emerging understanding, finding that, generally, no single model performs consistently best, but rather that individual model performances vary with the setting.

The model structure represents a formalized perception of how the catchment system is organized and how the various parts are inter-connected (Blöschl *et al.* 2008). Selection of a suitable model structure ideally depends on a number of factors as one strives to represent the runoff processes in a realistic way, so that the model can be safely used in a predictive mode. However, the level of detail with which this is done varies widely. Blöschl *et al.* (2013) identified three groups of information that can be used to guide model structure selection in view of process fidelity: *a priori* perception of processes, field data and reading of the landscape, and transferring the model structure from similar gauged catchments. Additional considerations in selecting a model structure are the modelling purpose (e.g. operational *vs* investigative models), data availability (more complex models require larger data availability), resource constraints (simpler models with lower budgets), and the modeller's experience (choosing models one has experience with). However, as emphasized by many authors, including Clark *et al.* (2011b), ambiguities in the choice of model structure have led to a plethora of models, and the community has struggled to identify the "most appropriate" models even in the relatively simple terms of "best empirical performance", let alone in terms of their scientific validity. The ongoing debate of how to best represent catchment processes can thus be seen as a symptom of an insufficient scientific understanding of hydrological processes at multiple scales. On the one hand, this is partly rooted in difficulties in appropriately measuring and representing the heterogeneity encountered in natural systems (McDonnell *et al.* 2007, Clark *et al.* 2011b), and thus to adequately answer the "closure" problem at the catchment scale (Reggiani *et al.* 1998, 1999, Beven 2006a, Harman *et al.* 2010). On the other hand, the proliferation of hydrological models is also clearly linked to the lack of a holistic hydrological theory (Sivapalan 2005, Troch *et al.* 2009a). Thus, in response to the limitations of universally applicable approaches, calls for more flexible approaches to modelling, allowing consistent comparison and testing of alternative model hypotheses (e.g. Beven 2000, McDonnell 2003, Pomeroy *et al.* 2007, Clark *et al.* 2008, Savenije 2009, Clark *et al.* 2011b, Fenicia *et al.* 2011) found increasing support during the PUB Decade.

Probably the first, widely communicated flexible modelling framework was the Modular Modeling System (MMS), introduced by Leavesley *et al.* (1996) and consisting of a module library and a GIS interface, allowing the design of user-selected model structures. The main purpose of the MMS was to link different modules aimed at representing different catchment compartments to constitute an integrated system model. In this respect, it may be useful to differentiate between "model-interfacing frameworks" and "flexible process representation frameworks" depending on the model "granularity" and underlying rationale (see Fenicia *et al.* 2011, for a discussion). Subsequently, the Rainfall–Runoff Modelling Toolbox (RRMT) with the associated Monte-Carlo Analysis Toolbox (MCAT) offered a choice of predefined conceptual soil moisture accounting modules and routing components that could be combined in different set-ups, thus allowing the modeller some freedom in customizing the model to catchment characteristics (Wagener *et al.* 2001, 2004).

Originally designed as a model diagnosis tool, the Framework for Understanding Model Structural Errors (FUSE) was introduced by Clark *et al.* (2008). In a quest for a better understanding of the differences between model structures and their respective suitability for differential boundary conditions, FUSE uses individual model components of four existing conceptual hydrological models—PRMS (Leavesley *et al.* 1983), NWS Sacramento (Burnash *et al.* 1973), TOPMODEL (Beven and Kirkby 1979) and ARNO/VIC (Zhao 1977)—as independent building blocks which can be freely reassembled to customized model architectures. As an extension to the FLEX modelling framework (Fenicia *et al.* 2006, 2008a), which is a more generic approach, Fenicia *et al.* (2011) presented a unified modelling platform for conceptual hydrological modelling, SUPERFLEX, based on generic building blocks, such as reservoirs, junctions and constitutive functions. Using combinations of these components, tailor-made model architectures can be developed and tested for suitability. With a strong focus on snow accumulation and ablation processes, and frozen soil behaviour in the context of both cold and warm season hydrology, similar to the Hydrograph model (Vinogradov *et al.* 2011, Semenova *et al.* 2013), Pomeroy *et al.* (2007) devised a modular modelling framework, the Cold Regions Hydrological Model (CRHM), allowing the user to adapt the ensemble of represented processes to correspond to the particular requirements of individual catchments. Similar to the MMS (Leavesley *et al.* 1996), the CRHM does not require much parameter calibration. The CRHM also permits internal algorithm and parameter set intercomparison, and model falsification through use of parallel model structures. Further frameworks that allow the integration of model components include the Land Information System (LIS; Kumar *et al.* 2006) and the Noah Land Surface Model with multiparameterization options (Noah-MP; Niu *et al.* 2011).

Linking these flexible modelling frameworks to the wide body of literature suggesting that different landscape types entail distinct hydrological functions (e.g. Andréassian 2004, Buttle *et al.* 2005, Oudin *et al.* 2008b), and that changes in the landscape can considerably influence the hydrological regime of catchments (e.g. Hundecha and Bárdossy 2004, Moore and Wondzell 2005, Samaniego and Bárdossy 2006, Alila *et al.* 2009, Yang *et al.* 2012), implicitly commands that, ideally, the most suitable model structure identified for a catchment should bear a conceptual resemblance to the modellers' perception of the system, reflecting the dominant processes at a specific location (e.g. Gan and Burges 1990a, Ambroise *et al.* 1996b, Beven and Freer 2001a, Pomeroy *et al.* 2005, Ye *et al.* 2012, Fenicia *et al.* 2013). This is also echoed by the dominant runoff process concept (DRP; Grayson and Blöschl 2000) and the development of suitable decision schemes, permitting the identification of distinct hydrological response units (HRU) based largely on geological, pedological and topographical considerations (Scherrer and Naef 2003, Pomeroy *et al.* 2007, Scherrer *et al.* 2007, Schmocker-Fackel *et al.* 2007). The distinct hydrological function of the individual response units then dictates the design of different model structures associated with them, thereby guiding model development (e.g. Uhlenbrook *et al.* 2004, Lindström *et al.* 2010, Hellebrand *et al.* 2011). In addition to applications of the HRUs in catchments with comparatively little anthropogenic disturbance, the concept also proved valuable for holistic representations of water fluxes in heavily human-modified environments, as demonstrated in recent examples (Efstratiadis *et al.* 2008, Nalbantis *et al.* 2011, Strömqvist *et al.* 2012). In a somewhat contrasting approach, rather than explicitly defining hydrological function, GIUH models (Rodriguez-Iturbe and Valdes 1979) interpret hydrological behaviour of the stream network by means of Horton ratios, while the width function instantaneous unit hydrograph models (WFIUH; Surkan 1969, Kirkby 1976, Beven 1979, Naden 1992, Rinaldo and Rodriguez-Iturbe 1996, Rodríguez-Iturbe and Rinaldo 1997) make use of response time distributions obtained from physically-based flow velocity parameters, thereby incorporating process heterogeneity, which was shown to be a valuable tool in ungauged environments (e.g. Moussa 2008, Grimaldi *et al.* 2010, 2012a, 2012b).

In a further development, Savenije (2010) explicitly invoked the self-organizing nature of catchments and the fact that flow paths have to reflect the dynamic equilibrium between drainage and storage functions of a catchment, pointing out the potential of landscape-driven modelling. In other words, as a result of the co-evolutionary nature of topography, ecosystem and hydrology, catchments need to store certain amounts of water, while still allowing efficient drainage, for the present vegetation and/or topography to have developed as they did (see Horton 1933, Sivapalan 2003b). Savenije (2010) further argued that catchments could be dissected in a semi-distributed way according to a hydrologically meaningful landscape classification metric that allows individual runoff processes to be assigned to different landscape units, thus enabling them to be associated with distinct hydrological functions such as can be explored in, for example, Dynamic TOPMODEL (Beven and Freer 2001). The proposed classification is not explicitly based on detailed catchment parameters as in the DRP approaches, but rather on the readily available Height Above the Nearest Drainage (HAND; Rennó *et al.* 2008, Nobre *et al.* 2011), which, according to Gharari *et al.* (2011), has the potential "*to meaningfully characterize landscapes as it originates directly from feedback processes between water and landscape and is* [. . .] *directly linked to the dominant driver of storage–discharge relationships: the hydraulic head*."

Going somewhat against the mainstream of flexible modelling approaches, data-based mechanistic modelling strategies (DBM; e.g. Young 1992, 2003, Alvisi *et al.* 2006, Ratto *et al.* 2007) proved highly valuable, in particular for real-time forecasting. Over the past decade, the growing importance of DBM, which, in contrast to the objectives of PUB, pays less attention to the physical interpretation of hydrological processes but rather focuses on the information content of data, is underlined by the development of "hydroinformatics" as an individual sub-discipline in hydrology. Data-based methods are also frequently used to characterize baseflow recessions via the construction of (non)linear master recession curves (e.g. Tallaksen 1995, Lamb and Beven 1997, Moore 1997, Wittenberg and Sivapalan 1999, Fenicia *et al.* 2006). Kirchner (2009) took the idea a step further and elegantly demonstrated that the complete rainfall–runoff response of a certain class of catchments (e.g. Teuling *et al.* 2010, Ajami *et al.* 2011, Birkel *et al.* 2011b) can be described as a simple first-order nonlinear system and the constitutive function generating their streamflow response can be directly inferred from observed streamflow fluctuations. This one-equation approach requires a maximum of four parameters, while resulting in comparable levels of performance to much more complex models. In addition, while compactly describing the water storage and release dynamics of catchments, the proposed approach can also be inverted to estimate spatially averaged precipitation and actual evaporation rates, in the light of the minimal parameterization, providing a strong test for the underlying theory. In a different approach, invoking long-range dependence (e.g. Koutsoyiannis 2002, 2005), the value of stochastic models for river flow prediction was underpinned by Koutsoyiannis *et al.* (2008b).

3.2.2 Exploiting new data in catchment models It was recognized early (Beven 1989a, Grayson *et al.* 1992, Jakeman and Hornberger 1993, Gupta *et al.* 1998) and strongly reiterated later (e.g. Gupta *et al.* 2008) that the predictive capability of hydrological models is limited by high model complexity relative to the typically low number of model constraints used to calibrate the models. In other words, models calibrated only to observed hydrographs can be considered over-parameterized if they consist of more than five parameters (Jakeman and Hornberger 1993). Widening the scope of hydrological models, requiring them to better reproduce multiple aspects of the system simultaneously, proved to be an important step forward (e.g. Kuczera 1983, Gupta *et al.* 1998, 1999, Vrugt *et al.* 2003, Samaniego and Bárdossy 2005, Bastidas *et al.* 2006, Yilmaz *et al.* 2008, Hughes 2010). An important strategy to reach this objective was the incorporation of orthogonal, sometimes "soft" forms of information, i.e. more qualitative data and often requiring some level of interpretation, in the modelling process. For example, Seibert and McDonnell (2002) reported that the inclusion of fuzzy measures of acceptability, e.g. for groundwater dynamics, resulted in significantly improved and more consistent overall model performances. Similarly, Freer *et al.* (2004) used fuzzy estimates of water table depth as additional calibration constraints to considerably reduce the number of feasible model parameterizations. Further "soft" and orthogonal information shown to be valuable for better process representation and more robust parameter estimation, in spite of the potential need for more parameters, included monthly water balance estimates (Winsemius *et al.* 2009), diatoms (Pfister *et al.* 2009), single (Vaché and McDonnell 2006, Dunn *et al.* 2007, Iorgulescu *et al.* 2007, Page *et al.* 2007, Son and Sivapalan 2007, Birkel *et al.* 2010b, Hrachowitz *et al.* 2013) and multiple tracer data (Meixner *et al.* 2002, Birkel *et al.* 2011a, Capell *et al.* 2012), as well as, on the way to integrated catchment models, combinations of tracer data with sub-catchment runoff (e.g. Uhlenbrook and Sieber 2005), groundwater dynamics (e.g. Fenicia *et al.* 2008a), or saturation area extent (e.g. Ambroise *et al.* 1996a, Birkel *et al.* 2010a). Assimilating remotely sensed data into catchment models is particularly relevant for predictions in otherwise ungauged basins. Nester *et al.* (2012a), for instance, demonstrated the value of remotely sensed snow cover patterns to constrain parameter uncertainty of catchment models. Others (Mohamed *et al.* 2006, Parajka *et al.* 2006, Winsemius *et al.* 2008) used remotely sensed soil moisture and evaporation, respectively, to improve model parameterizations. In contrast, Lerat *et al.* (2012) found that using catchment internal flow measurements as additional calibration targets provided only little model improvement. An example is given in Fig. 5 of how different data types, in this case of groundwater dynamics and stream tracer response, can enhance process representations in models. The progress in the use of multi-response field data thus not only enhanced the integrated understanding of dominant processes, but also guided the design and parameterization of integrated catchment models (see Ambroise *et al.* 1996b, Lindström *et al.* 2005, Clark *et al.* 2011a, McMillan *et al.* 2012b). Such robust representations of catchment internal process dynamics also increase the value of models for nutrient and contaminant transport studies (e.g. Molénat and Gascuel-Odoux 2002, Lyon *et al.* 2010b, Van der Velde *et al.* 2010, Arheimer *et al.* 2011, 2012, Strömqvist *et al.* 2012, Hrachowitz *et al.* 2013).

3.2.3 Advances in model calibration, testing and realism Hydrological models typically rely on calibration, traditionally done by minimizing some performance measure of the residuals between the

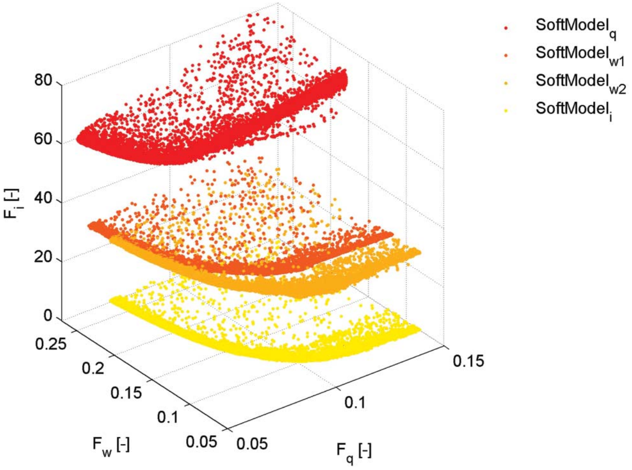


Fig. 5 Performance of a model with respect to streamflow (F_q), groundwater dynamics (F_w) and stream tracer response (F_i). Step-wise model improvements from the least complex SoftModel$_q$ (red) to the most complex SoftModel$_i$ (yellow) determine the orthogonal trajectory in objective space (from Fenicia *et al.* 2008a, © 2008 John Wiley and Sons).

observed and the modelled hydrograph, defined in terms of an objective function to be optimized. In the absence of an objective function that could give a global, generalized and comparable overall performance assessment of the hydrograph (or any other modelled variable), the choice of the objective function can have significant impacts on model results and parameterization (e.g. Sorooshian *et al.* 1983). The Nash-Sutcliffe Efficiency (NSE; Nash and Sutcliffe 1970) is one of the objective functions that became popular as a convenient and normalized measure of model performance. However, besides it being oversensitive to peak flows, due to the use of squared residuals (Legates and McCabe 1999), some studies have cast doubt on the usefulness of the NSE for comparative purposes (Seibert 2001, Mathevet *et al.* 2006, Schaefli and Gupta 2007). While McMillan and Clark (2009) suggested a modified version of NSE, Smith *et al.* (2008) introduced decomposed performance measures that individually account for bias, variability and correlation. Reflecting this work, Gupta *et al.* (2009) introduced the Kling-Gupta Efficiency (KGE), similarly based on a decomposed analysis of the form of the NSE. They showed that, when maximizing NSE, the variability in the modelled flows necessarily underestimates the variability in the observed flows (or corresponding target model output), a tendency that KGE is able to avoid. Criss and Winston (2008), however, argued that replacing NSE with a volumetric efficiency (VE) avoids the overemphasis of peak flows. In contrast, methods based on weighting different parameterizations for low- and high-flow periods (Oudin *et al.* 2006a) or different calibration objectives (Fenicia *et al.* 2007b) allow a balanced representation of the hydrograph. A further recently suggested objective metric, Series Distance, is based on an overall agreement of event occurrence as well as on amplitude and timing, bringing automated calibration techniques closer to visual hydrograph inspection (Ehret and Zehe 2011, Ewen 2011).

Notwithstanding the modifications of old and the design of new objective functions, Krause *et al.* (2005) found, from a comparative study with a suite of performance measures, that many of the tested performance measures exhibited no, or sometimes even inverse, correlations with each other, concluding that combinations of contrasting objective functions should be used for model calibration to ensure a balanced model parameterization. This strongly reflects early calls for multi-objective calibration efforts (Gupta *et al.* 1998, Madsen 2000). Complementing the benefits of multiple kinds of (orthogonal) calibration data, the value of multi-objective calibration has been recently corroborated in a variety of studies (e.g. Freer *et al.* 1996, Boyle *et al.* 2000, 2001, Madsen 2003, Vrugt *et al.* 2003, Engeland *et al.* 2006, Fenicia *et al.* 2007a, Parajka *et al.* 2007b, Moussa and Chahinian 2009, Hrachowitz *et al.* 2013), suggesting that it can produce robust parameterizations, more consistently representing the ensemble of real-world processes underlying the hydrological response. In addition, it was recognized that multi-objective calibration facilitates the detection of model structural failures (Gupta *et al.* 1998, 2008, Dornes *et al.* 2008b, Efstratiadis and Koutsoyiannis 2010). Moreover, the trade-offs in performance and the resulting Pareto optimal set of non-dominated solutions make it difficult to objectively decide on the most adequate parameterization for a model (see Schoups *et al.* 2005). However, Boyle *et al.* (2000) showed that this problem can be reduced by the incorporation of additional conceptual constraints to narrow down the selection. Further, Kollat *et al.* (2012) showed that trade-offs can collapse to well-identified single solutions when limiting the objective function estimates to meaningful precisions.

Closely related to multi-criteria and multi-objective calibration strategies is the growing understanding that, in the presence of data and model structural uncertainty, mathematically optimal parameterizations may be considerably different from hydrologically optimal solutions, which are more realistic process representations. In addition, data errors are likely to be different for different calibration periods, resulting in Pareto optimal solutions of one calibration period being potentially different from Pareto optimal solution of other calibration periods. This therefore dictates the need for incorporating uncertainty in the calibration process and for stringent model realism checks (Wagener 2003, Beven 2006a, McGuire *et al.* 2007, Gupta *et al.* 2008, Martinez and Gupta 2011, Andréassian *et al.* 2012).

Exhaustive and systematic model and data testing should thus play a critical role in filtering out both unrealistic parameterizations and unsuitable model structures. This was already recognized by Klemeš (1986), who made a convincing case for establishing a culture of systematic model testing. In spite of emphatic reiterations of the wider implications of this issue (Wagener 2003, Kirchner 2006, Andréassian *et al.* 2009, Martinez and Gupta 2011), the full model-testing procedure as suggested by Klemeš (1986), or similar schemes, were rarely applied (e.g. Refsgaard and Knudsen 1996, Donnelly-Makowecki and Moore 1999, Young 2006), and no standard protocols and procedures for model testing have so far become good practice in mainstream hydrology. This is in spite of the availability of testing frameworks and tools, such as the Generalized Likelihood Uncertainty Estimation (GLUE; Beven 2002, Beven *et al.* 2012), or the Dynamic Identifiability Analysis (DYNIA; Wagener *et al.* 2003), which is implemented in the MCAT (Wagener *et al.* 2004, Wagener and Kollat 2007). A formalized procedure for model development, testing and evaluation, i.e. for identifying behavioural models, was suggested by Jakeman *et al.* (2006), and combined model calibration–testing approaches were recently proposed by Coron *et al.* (2012) and Gharari *et al.* (2013), providing an objective way to better exploit the information content of streamflow time series in allowing the selection of sub-optimal but hydrologically feasible and time-consistent model parameterizations.

Resulting from the need for more rigorous model testing methods, the potential of different hydrological signatures, reflecting the functional behaviour of the catchment that a model should be able to reproduce, to serve as a link between process understanding and models (Jothityangkoon *et al.* 2001, Eder *et al.* 2003, Gupta *et al.* 2008, Carrillo *et al.* 2011, Clark *et al.* 2011b, Wagener and Montanari 2011, McMillan *et al.* 2012b) has recently received significant attention. A realistic model should thus not only be capable of satisfying different objective functions for various modelled variables, i.e. multi-objective and multi-criteria calibration, but should simultaneously also reproduce contrasting signatures of the hydrological response, thereby ensuring a resemblance in the functional behaviour and the statistical properties of observed and modelled variables (Fig. 6). The main advantage is that signatures focus the model calibration process on matching actual catchment behaviour in a meaningful way and therefore have a chance of leading to

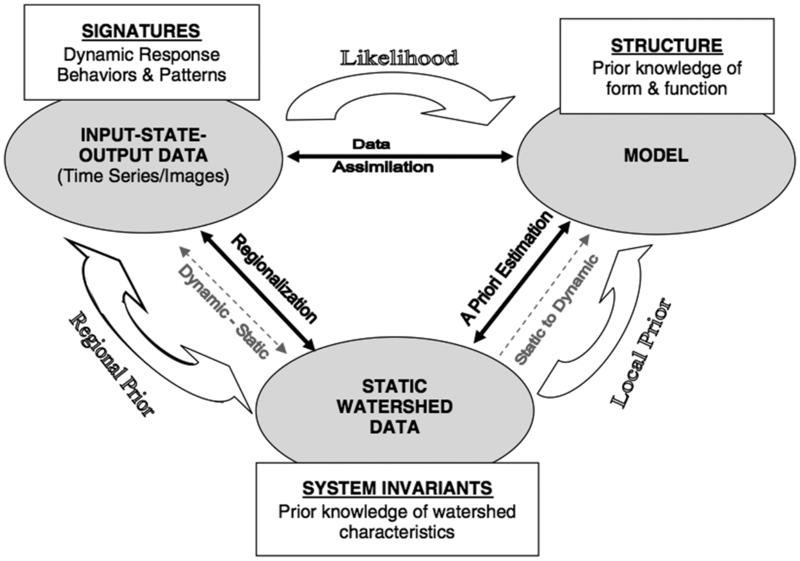


Fig. 6 Three types of information available for constraining a predictive model (from Gupta *et al.* 2008, © 2008 John Wiley and Sons, Ltd.).

models with more realism. Furthermore, the use of different signatures can reduce the impact of input data errors during the calibration procedure. Some of the suggested signatures that have proved useful for model evaluation are the flow duration curve (Yadav *et al.* 2007, Yilmaz *et al.* 2008, Westerberg *et al.* 2011b), the baseflow index (Bulygina *et al.* 2009), the rising limb density (Shamir *et al.* 2005, Yadav *et al.* 2007), the peak distribution (Sawicz *et al.* 2011) and the spectral density of runoff (Montanari and Toth 2007, Winsemius *et al.* 2009), while Schaefli and Zehe (2009) evaluated their model in the wavelet-domain.

It is recognized that in many poorly gauged regions there is an almost complete lack of streamflow observation with which to undertake calibration and testing. For these regions, calibration and regionalization are simply not possible. However, in sparsely gauged regions there are streamflow measurements which can provide important information on catchment behaviour, and the interest is in increasing the value of these measurements for prediction in the adjacent ungauged catchments. A question related to that notion: Which observation data length is necessary to obtain adequate model parameterizations? was raised and investigated long before the PUB Decade (e.g. Ibbitt 1972, Sorooshian *et al.* 1983, Gupta and Sorooshian 1985, Yapo *et al.* 1998) and further explored by Xia *et al.* (2004). It was concluded that different observation data lengths are necessary for different parameters to be determined adequately. In a detailed analysis, Vrugt *et al.* (2006) showed that 2–3 years of streamflow data are sufficient to obtain robust parameter estimates for the SAC-SMA model. A similar result was obtained by Kuchment and Gelfan (2009), who applied a distributed physically-based model for catchments located in the arid steppe and permafrost regions. However, Merz *et al.* (2009) argued that more than 5 years of calibration period may be necessary to obtain stable parameter estimates in humid temperate climates. Other studies highlighted the potential of using only a few, well-chosen observations, preferably including unusual events to identify robust and stable parameterizations (Rojas-Serna *et al.* 2006, Seibert and Beven 2009, Singh and Bárdossy 2012). Perrin *et al.* (2007) further pointed out that low complexity models need fewer data to constrain the feasible parameter space and that stable parameterizations are more problematic to obtain in catchments characterized by dry climate than in humid climates. In general it should be noted that the conclusions of the above studies need to be seen not only in terms of data quantity but also in terms of the quality of available data (see Beven and Westerberg 2011).

3.2.4 Advances in model uncertainty assessment During the PUB Decade increasing awareness developed in the community that uncertainty analysis needs to take on a more prominent position in hydrology (Beven 2008). Comprehensive end-to-end uncertainty analysis (e.g. Pappenberger *et al.* 2005, Nester *et al.* 2012b) is instrumental in avoiding potential interpretative pitfalls, as it puts analysis results on a more robust scientific basis, while also allowing closer appraisal of the influence of different error sources on model quality (Dunn *et al.* 2008). Thus, in spite of a variety of common arguments against uncertainty assessment, as discussed by Pappenberger and Beven (2006), not only should uncertainty analysis be an integral part of a scientific paper (Beven 2006b), but it should also be systematically implemented according to a general Code of Practice, rather than on an *ad hoc* basis (Pappenberger and Beven 2006, Wagener *et al.* 2006, Liu and Gupta 2007).

However, due to the inevitably difficult interpretation of “uncertain” results, strategies are necessary to unambiguously communicate such uncertain predictions to users and decision makers, as stressed by Beven (2007). Likewise, others pointed out the need to better define, understand and communicate the basis of uncertainty (Montanari 2007, Todini and Mantovan 2007).

Although considerable progress has been made and the need for more rigorous uncertainty analysis is now widely accepted, there is on-going discussion about the most suitable techniques to use (Liu and Gupta 2007, Montanari *et al.* 2009), and on the consistency of the uncertainty bounds provided by different techniques. In the light of imperfect model structures, non-stationary errors in input data and the complex structure of model residuals, Beven and Freer (2001b), as well as Beven (2006b, 2006c, 2008), argued that the GLUE model (Beven and Binley 1992) is an effective uncertainty analysis technique. Due to subjectivity in the choice of behavioural models (Montanari 2005) and its use of non-formal likelihoods that are inconsistent with probability theory, GLUE is met with scepticism (Mantovan and Todini 2006, Todini and Mantovan 2007, Stedinger *et al.* 2008, Montanari *et al.* 2009, Clark *et al.* 2012), although, in further developments of GLUE, observational uncertainties are more explicitly taken into account to derive “limits of acceptability” and reduce subjectivity (e.g. Beven 2006c, Liu *et al.* 2009). Parts of the community thus consider Bayesian techniques to be more appropriate as formal statistical methods for uncertainty analysis (Kavetski *et al.* 2002, Vrugt *et al.* 2003, Schoups *et al.* 2010). In spite of methods reducing the non-stationarity of error structures and developments of advanced error models (Thyer *et al.* 2009, Schoups and Vrugt 2010), Beven *et al.* (2008) argued that formal likelihood measures can be highly problematic, suggesting that even small deviations from the required assumptions can result in model over-conditioning and inadequate parameterizations. This can only be avoided if all sources of uncertainty can be treated as aleatory, i.e. random in nature (Westerberg *et al.* 2011b, Beven 2013), thus if the residuals converge towards the true prediction uncertainty distribution (Beven and Westerberg 2011). Treating non-stationary, epistemic uncertainties, i.e. errors due to lack of knowledge (Beven 2013) as aleatory will result in over-conditioning of posterior parameter distributions and thus underestimation of uncertainty, especially in the presence of disinformative data, strongly indicating the need to separate these two error types (Beven *et al.* 2011, Beven and Westerberg 2011, Beven 2013, Gong *et al.* 2013). Andréassian *et al.* (2007), however, made the intriguing case that both uncertainty frameworks, i.e. GLUE and Bayesian methods, are potentially underestimating the scale of the problem.

Kuczera *et al.* (2006) showed that lack of good prior information on the different sources of uncertainty creates an ill-posed problem, and that it is difficult to reliably disentangle the different sources of uncertainty, potentially resulting in disproportional effects on the modelled results (Kuczera *et al.* 2010). They concluded that the availability of a rainfall–runoff record alone is insufficient to disentangle the different sources of error. Subsequent work (Renard *et al.* 2010, 2011) suggests that disentangling different types of errors is more tractable when stronger independent, prior information, such as results of geostatistical analysis, is available. The importance of separating different sources of uncertainty was further underlined by Beven and Westerberg (2011). Doubting the general information content of data, they argued that disinformation in data can introduce considerable and potentially long-lasting effects on model results and parameterizations, which could partly explain difficulties to adequately model certain catchments.

Although the combined importance of model structural, parameter and data errors are by now widely accepted in the community, decomposing the different sources of error has proven comparatively difficult, although a wealth of studies attempted to address the topic during the PUB Decade. In detailed analyses (e.g. Andréassian *et al.* 2001, Oudin *et al.* 2006a), it was shown that model performance and parameterization are highly sensitive to both random and systematic errors in precipitation data (e.g. Hrachowitz and Weiler 2011). These conclusions are supported by the results of Kavetski *et al.* (2006a) and Renard *et al.* (2011) using the Bayesian Total Error Analysis (BATEA) tool and by Vrugt *et al.* (2008) using the Differential Evolution Adaptive Metropolis (DREAM) algorithm. In spite of obtaining a better understanding of the effects of input error, it was also demonstrated that detailed insights into model structural errors are hampered by insufficiently specified error models (Kavetski *et al.* 2006a), which was later addressed by Renard *et al.* (2011). McMillan *et al.* (2011b) further showed that multiplicative error formulation for precipitation based on lognormal distributions can approximate true error characteristics, albeit somewhat misrepresenting the distribution tails. Interestingly, and in contrast to precipitation, it was found that models are relatively insensitive to errors in potential evaporation series, most likely due to the buffering capacity of the soil moisture components and the related low-pass filter properties of models (Andréassian *et al.* 2004a, Oudin *et al.* 2004, 2005a, 2006a). It was nevertheless shown that the use of relatively simple temperature-based methods to estimate potential evaporation leads to somewhat better model performances than the use of the Penman approach (Oudin *et al.* 2005b).

Likewise, streamflow data can exhibit considerable uncertainties as a result of the combined influences of erroneous stage or velocity measurements, insufficient numbers of individual gaugings and changes in river cross-sections, leading to non-stationary stage–discharge relationships (e.g. Sorooshian and Gupta 1983, Di Baldassarre and Montanari 2009, McMillan *et al.* 2010, Westerberg *et al.* 2011a). In an attempt to consider the uncertainty in streamflow in models, for instance McMillan *et al.* (2010) proposed a method to generate a streamflow error distribution which can be used to form a likelihood measure for model calibration (see also Liu *et al.* 2009, Krueger *et al.* 2010). An example application of the method is shown in Fig. 7.

Different further approaches were introduced for an improved treatment of data, model structure and parameterization errors in model calibration.

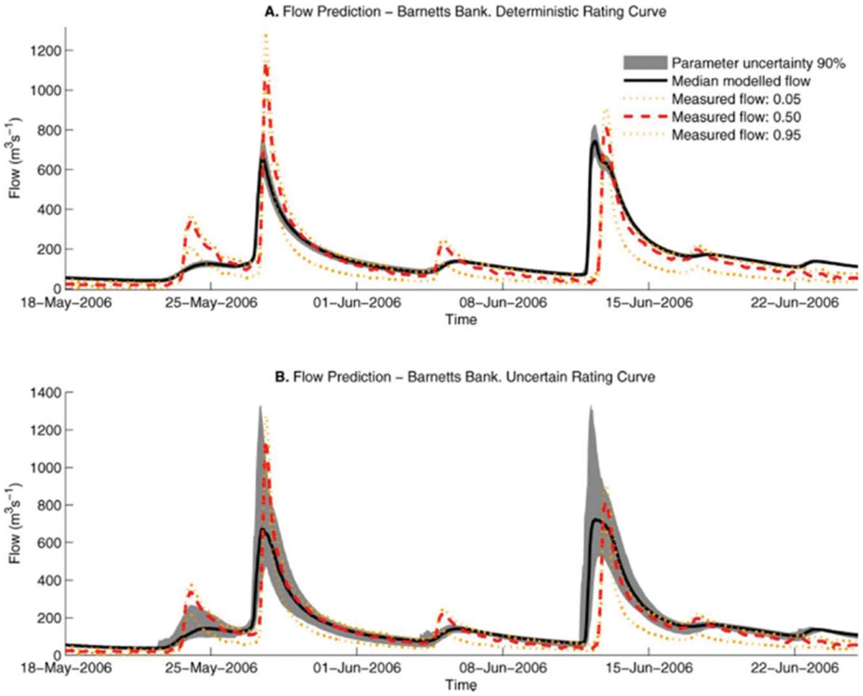


Fig. 7 Example of a modelled hydrograph (90% confidence interval) based on calibration using (a) a deterministic rating curve and (b) a rating curve including uncertainty (from McMillan *et al.* 2010, © 2010 John Wiley and Sons, Ltd.). This result illustrates the effect of rating curve uncertainty, which may add uncertainty to model predicitions, especially for estimating extremes.

While Vrugt *et al.* (2005) demonstrated the utility of combined global optimization and data assimilation for improved estimates of parameter and prediction uncertainty, Bárdossy and Singh (2008) identified robust parameterizations based on an analysis of stochastically generated synthetic data errors. Various studies have presented methods to simultaneously and explicitly account for errors from different sources (e.g. Götzinger and Bárdossy 2008, Krueger *et al.* 2010). However, Gupta *et al.* (2012) pointed out that model structural adequacy errors are of several types (perceptual, conceptual physical, conceptual process, spatial variability, equation and numerical) arising at different steps in the modelling process, and that a detailed study of these various causes is necessary to ultimately address issues of learning by the process of confronting models with data (Gupta *et al.* 2008, see also Section 3.2.5). However, as emphasized by Kumar (2011) and Wagener and Montanari (2011), additional challenges for predictability that are not yet well understood arise, for example, from dynamic changes in the spatial complexity of the system. Offering an alternative approach to treating uncertainty, Montanari and Koutsoyiannis (2012) stochastically perturbed data, model parameters and output in a multi-model approach, accepting that "*uncertainty is an intrinsic property of nature, and that causality implies dependence of natural processes in time*" (Koutsoyiannis 2010), which in principle implies a predictable system. Pursuing this argument, even small uncertainties, e.g. in the initial conditions, may result in unpredictability. It is thus desirable and possible to "*shape a consistent stochastic representation of natural processes, in which predictability (suggested by deterministic laws) and unpredicitability (randomness) coexist and are not separable or additive components*" (Koutsoyiannis 2010).

A further aspect of uncertainty was pointed out by Kavetski *et al.* (2006b), who argued that problems related to calibration, such as complex structures on objective function response surfaces, are not necessarily characteristics of models themselves, but rather are partly artefacts arising from inappropriate numerical implementation. In other words, in the absence of analytical solutions for the partial differential equations featuring most hydrological models, numerical approximations can result in inconsistent and biased model parameterizations. In detailed analyses, it was shown that commonly applied fixed-step explicit methods are unsuitable for use in hydrological models, and the community was encouraged to reconsider this aspect and call for more appropriate techniques, such as adaptive time stepping or implicit methods (Clark and Kavetski 2010, Kavetski and Clark 2010, Schoups *et al.* 2010). Similarly, low temporal data resolution may not only lead to the identification of unsuitable model structures (e.g. Arnaud *et al.* 2002, Zehe *et al.* 2005, Michel *et al.* 2006), but can also cause spurious parameter estimates (Hrachowitz *et al.* 2011a, Kavetski *et al.* 2011). This issue can only partly be solved by robust numerics. Where, for example, there is a mismatch between the information content of input data, output data and information used in the model, methods of interval arithmetic can help to provide more robust parameter estimates (Van Nooijen and Kolechkina 2012).

Notwithstanding the significant advances in model uncertainty assessment discussed above, Wagener and Montanari (2011) pointed out that the focus needs to shift from reducing model uncertainty towards reducing the uncertainty in our understanding of how catchments function under given environmental boundary conditions, as this holds the key to developing more reliable predictions in ungauged basins. This critical point of linking catchment form to hydrological function in order to reduce predictive uncertainty in ungauged basins largely depends on knowledge synthesis via comparative hydrology. In other words, rather than constraining model structural and parameter prior distributions, based on some knowledge of the system (see Section 3.3.1), it can prove valuable to infer information on the functioning of an ungauged catchment, for example, in the form of regionalized hydrological signatures (i.e. metrics describing different response characteristics of a catchment, such as the flow duration curve) and to train the model in the ungauged catchment to reproduce these signatures. Thereby, the feasible model and parameter spaces can be constrained and estimates for predictive uncertainty can be derived from the ensemble of retained behavioural models. This approach was successfully adopted by several authors. Yadav *et al.* (2007) regionalized the slope of the flow duration curve, high pulse counts and baseflow index, including their respective prediction limits on the basis of regression models. By forcing models to reproduce these signatures so as to fall within the respective prediction bands, they were able to significantly constrain the feasible parameter space and thereby reduce the predictive uncertainty of their models. This approach was refined by Zhang *et al.* (2008), who introduced a multi-objective framework to identify feasible parameterizations for ungauged basins. In a somewhat different vein, not relying on regionalized information, but rather on scarce information on the catchment of interest itself, Winsemius *et al.* (2009) were able to constrain the prior parameter distributions and to narrow prediction intervals by discarding parameterizations that could not reproduce the estimated shape of the recession, the spectral properties and the monthly water balance (Fig. 8). Other examples for similarly deriving constrained posterior distributions and reducing predictive uncertainty in ungauged basins include the use of the baseflow index estimated from soil types (Bulygina *et al.* 2009, 2011), satellite observations of flood extent (Di Baldassarre *et al.* 2009), and the use of parameter libraries derived from model parameterizations of a large set of gauged catchments (Perrin *et al.* 2008, Kuchment and Gelfan 2009).

A more holistic approach of comparative uncertainty quantification has been adopted by Blöschl *et al.* (2013). Predictive uncertainty was estimated by the cross-validation performance of the prediction of runoff signatures, in the form of blind testing. This comparative assessment is a way of assessing predictions and estimating model uncertainty through an ensemble of predictions in different places (Andréassian *et al.* 2006). It includes all sources of uncertainty, such as input data, model structure and parameters (Wagener and Montanari 2011). In contrast to traditional approaches, there is no error propagation involved. Instead, cross-validation performance is used as an estimator of total uncertainty. One of the generic findings of a comparative analysis of 25 000 catchments around the world was that uncertainty tends to increase with aridity and decrease with catchment scale. The comparative framework therefore facilitated pattern identification, and holds a lot of promise for complementing traditional uncertainty approaches, as well as for harmonizing hydrological research in both gauged and ungauged basins.

3.2.5 The potential of models as learning tools In the light of advances in model design and uncertainty analysis, the potential of models to teach us more about the system can and should be thoroughly exploited by using models as learning tools, as stressed by Beven (2007) and Dunn *et al.* (2008). This refers to testing different model structures and treating them as multiple working hypotheses, for a given catchment (e.g. Clark *et al.* 2011b). Rigorous model testing can then not only reveal model weaknesses but, in a feedback process, can also inform the modeller as to which parts of the hydrograph are not well reproduced by a given model (Savenije 2009), thereby

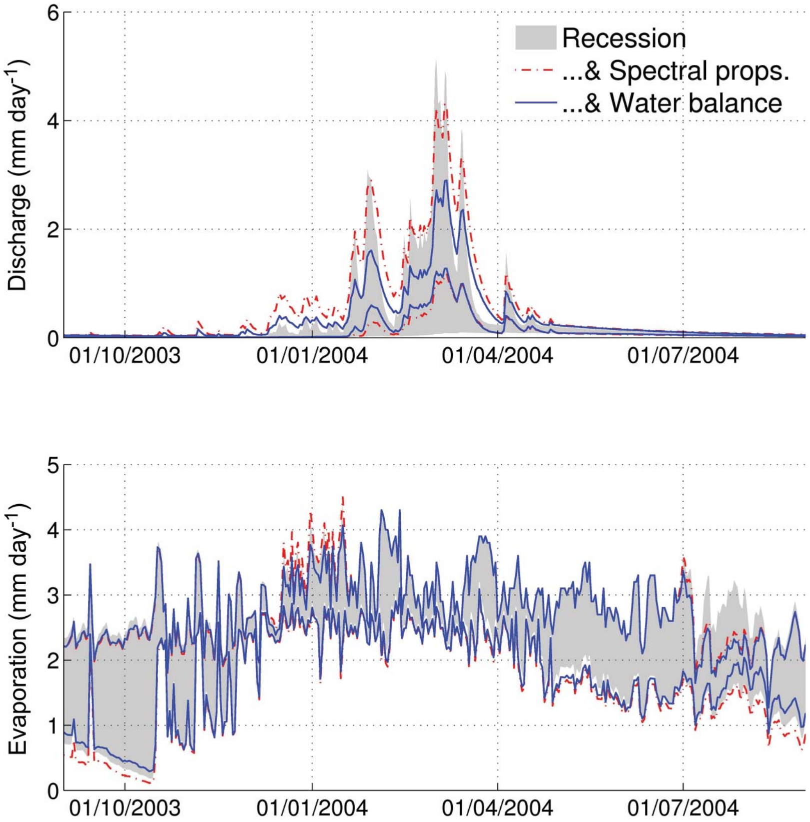


Fig. 8 The 5% and 95% plausibility intervals of output based on posterior parameter distributions with multiple constraints (recession slope, spectral properties, monthly water balance): discharge (top) and evaporation (bottom, from Winsemius *et al.* 2009, © 2009 John Wiley and Sons, Ltd.). This example illustrates the potential value of applying constraints based on "soft" data and emergent properties, to reduce predictive uncertainty especially for predictions in data-scarce regions.

guiding model improvement and resulting in better process understanding (Kavetski and Fenicia 2011, Martina *et al.* 2011, McMillan *et al.* 2011a, Fenicia *et al.* 2013). For example, Reusser *et al.* (2009) used a data-reduction method based on self-organizing maps to identify the timing of different dominant error types, which can inform the modeller about model structural errors. In a quite different approach, Bulygina and Gupta (2009, 2010, 2011) demonstrated the utility of Bayesian data assimilation as a strategy for detecting, diagnosing and correcting model structural errors. Analysing and evaluating models for periods of high information content and, thus, the typically non-stationary identifiability of individual parameters (Wagener *et al.* 2003, Wagener and Kollat 2007, Reusser *et al.* 2011) is also an extremely valuable task for learning more about the system and the impact of change on the system (e.g. Buytaert and Beven 2009, 2011, Merz *et al.* 2011).

Arguing that current model testing strategies are largely inadequate and that much more information could be extracted from data and models, Gupta *et al.* (2008) proposed a robust evaluation scheme based on hydrological signatures. Such an evaluation scheme would allow a more comprehensive assessment of different relevant system dynamics and thus enable us to use models to increase our knowledge and to enhance our perception of the system. Similarly, Euser *et al.* (2013) designed a framework that allows a multi-dimensional evaluation of different model hypotheses based on a range of hydrograph signatures.

The notion of models as learning tools can be extended by assuming that a given, well-tested model is a suitable representation of real-world processes. In fact, such a model can be used not only to infer the importance of different processes and boundary conditions in a given catchment (e.g. Gelfan *et al.* 2004, Grimaldi *et al.* 2010, Nippgen *et al.* 2011), but also, in a much broader sense, to serve as a virtual reality for experiments, from which, in turn, response patterns and internal system dynamics, as well as their sensitivity to changing boundary conditions and climatic forcing, can be explored and compared. Bashford *et al.* (2002), as well as Weiler and McDonnell (2004), for example, sought to understand the value of different data and to improve process conceptualizations with virtual experiment approaches. In a subsequent paper, Weiler and McDonnell (2006) demonstrated the utility of virtual experiments to quantify first-order controls, such as drainable porosity and soil depth variability, on nutrient transport. Dunn *et al.* (2007) used the concept to learn more about how catchment boundary conditions, such as mixing storage, influence water mean residence time, while Hrachowitz *et al.* (2013) used models in a virtual experiment approach to track water and tracers through the system in order to analyse the climatic controls on the dynamics of water age distributions. Their main finding was that water age distributions depend on model complexity as well as on mixing mechanisms, and they can exhibit substantial hysteresis effects, reflecting antecedent conditions. In a somewhat contrasting application of the virtual experiment concept, Kling and Gupta (2009) evaluated the effect of insufficient representation of spatial variability in a catchment on the optimal parameter values. They found that, when ignored in a model representation, spatial variability of physical catchment characteristics can generate considerable noise in the parameter estimates, depending on model complexity and parameter interactions.

Models, however, can also serve as valuable learning tools in ungauged catchments, when combining regionalized information of catchment function or our expectation of the catchment behaviour, i.e. hydrological signatures, with model priors, i.e. the model's uncertain prediction of the catchment behaviour, as emphasized by Wagener and Montanari (2011) and demonstrated by a comparative modelling study in an artificial catchment (Holländer *et al.* 2009). In other words, by constraining the parameter and model spaces with some metric of expected catchment behaviour, unfeasible representations of reality can be identified and discarded, thereby allowing the modeller, in a feedback process, to better understand the way a catchment functions. Ways to infer the expected behaviour of ungauged catchments are, for example, to regionalize specific hydrological signatures (see Section 3.3.1, e.g. Castellarin *et al.* 2004, Yadav *et al.* 2007, Bulygina *et al.* 2009, Pallard *et al.* 2009), or to use combinations of quantitative and qualitative information to derive limits of acceptability on specific signatures (e.g. Winsemius *et al.* 2009).

In addition to the benefits of using models as learning tools discussed above, this approach is crucial for guiding and improving experimental design to maximize the information to be gained from data. These examples highlight the potential of models as learning tools, an approach that is far from being exhaustively exploited and which may prove highly valuable for many future applications.

3.3 Catchment classification and new theory

Hydrological sciences are characterized by substantial process heterogeneity across places as well as spatial and temporal scales. For a long time this heterogeneity has impeded attempts to deepen our understanding of what controls hydrological processes and how they are linked. Yet, only from insights into the effects of these heterogeneities on response patterns, in other words, from a synthesis of process understanding, i.e. assembling individual pieces of information to search for an unknown pattern, valid across multiple spatial and temporal scales (see Thompson *et al.* 2011a), can a holistic theory of hydrology emerge (Sivapalan 2005, Blöschl 2006). The identification of scaling relationships, as well as the development of catchment classification schemes and similarity frameworks, based on comparative studies can be seen as a promising way forward towards synthesis (McDonnell and Woods 2004). Such a comparative approach was adopted in the PUB synthesis book (Blöschl *et al.* 2013) to organize the diversity of knowledge about runoff prediction. The approach sheds light on co-evolutionary processes of climate, geology, topography and ecology to understand catchments as complex systems (e.g. Gaál *et al.* 2012). Process relationships and generalizations can therefore be inferred, even for conditions and scales for which rigorous mechanistic models are not yet formulated.

3.3.1 Advances in process and parameter regionalization It is probably fair to say that scientific hydrology was highly fragmented at the beginning of the PUB Decade. It was soon realized that linking the results of individual process studies and designing designated comparative process and modelling studies (e.g. Andréassian *et al.* 2006, Carey *et al.* 2010) would prove highly instructive in exploring the overall patterns driving hydrological response, eventually facilitating process regionalization. This was one of the core objectives of the PUB initiative, as regionalization is instrumental for assessing and predicting hydrological response in ungauged catchments. Comparative studies were instrumental in identifying robust ways for regionalizing process knowledge. In general terms, regionalization efforts can be classified as (He *et al.* 2011): (a) direct regionalization of flow and flow metrics, and (b) regionalization of model parameters, both of which are based on either regression methods, or some kind of distance measures between gauged and ungauged sites.

Relatively simple regression approaches have already shown some value for determining first-order controls on catchment function in data-scarce regions. For example, in attempts to formulate parsimonious expressions for estimating mean annual flow, baseflow index and other flow metrics for data-scarce areas in Africa, Mazvimavi *et al.* (2004, 2005) compared 52 catchments, concluding that mean annual precipitation, land cover, mean catchment slope and drainage density are important controls on flow. Cheng *et al.* (2012), on the other hand, identified the baseflow index, a proxy for the combined influence of geology, soils, topography, vegetation and climate, as the dominant control on the shape of flow duration curves. Investigating flood frequency in 44 catchments, Pallard *et al.* (2009) were able to show the influence of drainage density. The influence of different landscape elements, characterized by distinct dominant processes, on functional patterns was demonstrated by Lyon *et al.* (2012) in a study based on 80 nested sub-catchments. As highlighted by Marechal and Holman (2005) in a simple regression approach, the British Hydrology Of Soil Types scheme (HOST), for example, is very robust for predicting the baseflow index, low flow statistics and the standard percentage runoff based entirely on soil map data. Other studies were able to establish similar links between stream chemistry and different flow paths (e.g. Laudon *et al.* 2007, Soulsby *et al.* 2007, Harpold *et al.* 2010), or climate (e.g. Dawson *et al.* 2011, Laudon *et al.* 2012).

Based on more complex regression models, low flows were regionalized with the use of a variety of seasonality indices, revealing the benefits of customizing regression models to regional requirements, rather than using global models (Laaha and Blöschl 2006a). In a subsequent analysis (Laaha and Blöschl 2006b), it was shown that regression models based on catchments grouped according to seasonality provide highly robust regionalization results. In a further example, applying a strong regional relationship with physical catchment characteristics, Soulsby *et al.* (2010b) were able to predict mean transit times, while, in a rather different type of study, they successfully used regression models to estimate flow metrics as a function of catchment mean transit time (Soulsby *et al.* 2010a).

Similarly, geostatistical methods have proven valuable for estimating hydrological variables in ungauged catchments. Skøien and Blöschl (2007), for instance, developed the topological kriging technique (or top-kriging), which accounts for hydrodynamic and geomorphical dispersion. Their results indicate that this technique can not only outperform deterministic runoff models in regions where stream gauge density is sufficiently high, as it avoids problems with input data errors and parameter identifiability, but also provides more robust estimates than regional regression models (Laaha *et al.* 2013). Comparison of top-kriging with Physiographical-Space Based Interpolation (PSBI) highlights the complementary utility of the two methods for headwater and larger-scale catchments (Castiglioni *et al.* 2011).

However, it is increasingly acknowledged that spatial, proximity does not necessarily entail similarity in functional behaviour (e.g. Ali *et al.* 2012), and that the efficiency of distance-based approaches can be considerably improved when applying some sort of hydrologically more meaningful distance measure (Bárdossy *et al.* 2005, He *et al.* 2011). For example, Merz *et al.* (2008) combined the top-kriging method with catchment characteristics to enhance the predictive performance of the method. An alternative method to assess functional similarity was introduced by Archfield and Vogel (2010). Instead of using the spatially closest stream gauge as reference for transferring daily flow to an ungauged site, they proposed the kriging-based map-correlation method, which selects the reference stream gauge whose flows are most correlated to the ungauged site. Likewise, pursuing the search for hydrologically more meaningful dissimilarity measures for predicting flow, Samaniego *et al.* (2010a) suggested the use of pair-wise empirical copula densities. For the prediction of long-term flow duration curves, Castellarin *et al.* (2007) tested and confirmed the utility of a stochastic index-flow model, while Castellarin (2007) demonstrated the use of probabilistic envelope curves for determining plausible extreme flood values in ungauged catchments.

In contrast to the regionalization of flow metrics, regionalization efforts for transferring model parameterizations from gauged to ungauged catchments have a longer tradition (see Wagener *et al.* 2004), despite the additional uncertainty introduced by input data and model structural errors, as well as the need for parameter calibration at the gauged sites (Wagener and Wheater 2006, He *et al.* 2011). Extrapolating their model parameters, Dunn and Lilly (2001) were among the first to explore the potential of parameter regionalization based on the HOST classification. In a subsequent comparative study, it was demonstrated that models run with HOST-derived parameter sets performed as well as independently calibrated models (Soulsby and Dunn 2003). In a similar way, a range of studies demonstrated the potential of soil data to guide *a priori* parameterizations of the SAC-SMA model, valuable for parameter regionalization with limited need for calibration (e.g. Koren *et al.* 2003, Smith *et al.* 2004, Anderson *et al.* 2006), thus underlining the value of hydrologically meaningful soil classification schemes (e.g. Boorman *et al.* 1995, Schneider *et al.* 2007). Other studies emphasized the value of parameter regionalization methods based on either physiographic similarity, as a proxy for functional similarity (Arheimer and Brandt 1998, Parajka *et al.* 2005, Dornes *et al.* 2008b, Masih *et al.* 2010), or spatial correlation, where gauge density is sufficiently high (Merz and Blöschl 2004, Oudin *et al.* 2008a). Figure 9 gives an example of such clear spatial patterns of calibrated parameters in a densely gauged region. Further, Parajka *et al.* (2007a) demonstrated that simultaneous calibration of model parameters (regional calibration) can be beneficial for runoff simulation in ungauged catchments. In fact, one of the strengths of the regional calibration method is to reduce the uncertainty of the estimated parameters. Extending the use of transfer functions and imposing conditions of monotony and uniform continuity on model parameters during calibration proved to be a significant improvement, as it resulted not only in adequate model performances but also in more consistent regression relationships (Götzinger and Bárdossy 2007). It was, however, also pointed out that the presence of equifinality in calibrated parameters limits the use of the methods discussed above for extrapolating individual parameters and that, instead, complete parameter sets should be transferred to ungauged sites (Bárdossy 2007). Addressing the issue of scale dependency of parameters, Samaniego *et al.* (2010b) proposed an elegant multi-scale parameter regionalization method to link finer resolution of input data to the coarser scale at which dominant processes are active. Similarly, step-wise methods have been proposed for simultaneous multi-basin calibration, including first headwaters of similar physiographic character, then river reaches and finally

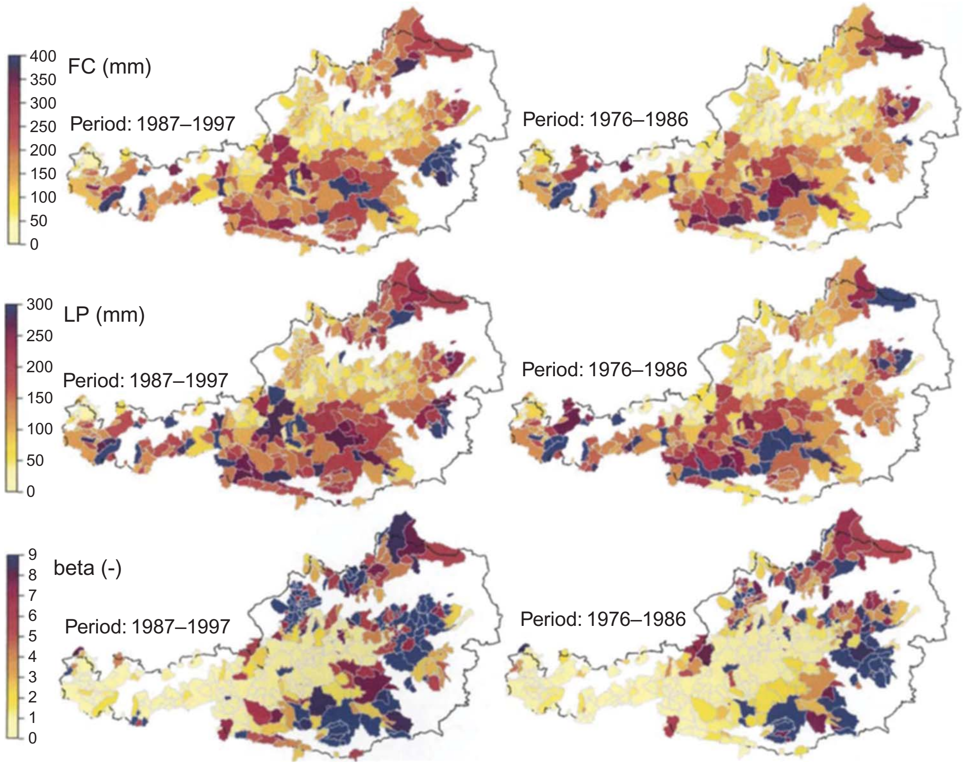


Fig. 9 Spatial patterns of selected calibrated model parameters—top: maximum soil moisture storage FC (mm); centre: potential evaporation limit LP (mm); and bottom: nonlinearity parameter β (-)—for the calibration periods 1987–1997 (left) and 1976–1986 (right) (from Merz and Blöschl 2004, © 2004 Elsevier). This illustrates the potential of using spatial proximity as a proxy for functional proximity in densely gauged regions.

lakes to find robust parameters across large regions (Arheimer and Brandt 1998, Donnelly *et al.* 2009, Arheimer *et al.* 2012, Strömqvist *et al.* 2012).

An alternative to parameter regionalization based on calibrated parameter sets at gauged sites is the use of direct *a priori* parameter estimation from measurable catchment physical property data (Hughes and Kapangaziwiri 2007). Kapangaziwiri *et al.* (2009, 2012) investigated the use of such methods, incorporating uncertainty, and compared the model outputs with uncertain regional signatures of catchment runoff response and groundwater recharge estimates. They found that there was little consistency in the results and, in some cases, the uncertain parameter estimates generated narrower uncertainty bounds than the regional signatures. However, Fang *et al.* (2010) demonstrated that the performance of a physically-based hydrological model using *a priori* parameters derived from a LiDAR DEM for an agricultural catchment was close to the that of a calibrated model, and that it was a good approach where detailed DEMs are available for ungauged catchments. Dornes *et al.* (2008b) emphasized that physically measurable parameters could be transferred thousands of kilometres if physically-based models were used and the ecohydrological similarity of catchment function could be assured. In a more recent study, Fang *et al.* (2013) have shown that appropriately structured flexible, physically-based models with *a priori* parameter estimation from measurements on site, or in similar conditions, can provide robust estimation of snowpack, soil moisture and streamflow at multiple scales, and that falsification of the model (CRHM) from appropriate structures leads to substantial model failure despite the use of measured parameters.

In a cross-over approach, Yadav *et al.* (2007) regionalized dynamic response characteristics of catchments based on physical characteristics. They subsequently used the extrapolated flow metrics to constrain model parameterizations at ungauged sites, thereby avoiding problems of model structural and parameter calibration errors. Blöschl *et al.* (2013) summarized how remotely sensed data, such as evaporation, soil moisture and snow patterns, can serve to constrain regionalized model parameterizations at ungauged sites. Notwithstanding the advances discussed, Oudin *et al.* (2010) pointed out that the frequent assumption of close correspondence between physical and functional similarity of catchments may be invalid in many catchments.

3.3.2 Advances in catchment classification and similarity frameworks A further important step towards the formulation of a holistic hydrological theory is the design of a generally accepted catchment classification framework, based on similarity of hydrological function, thereby providing a means to assess the dominant controls on patterns of water movement in catchments (McDonnell and Woods 2004). As discussed by Wagener *et al.* (2007), the ultimate goal of classification is to understand how catchment structure, climate and catchment function (i.e. response pattern) interact. Different types of classification are already in use, but fall short of providing a comprehensive picture of hydrological response patterns and causes of similarities between catchments. An effective classification scheme should thus be characterized by the ability to identify the ensemble of dominant factors causing the hydrological behaviour of a catchment, thereby combining “form”, i.e. the boundary conditions or structure of the system, and forcing, i.e. climate characteristics (see Winter 2001). Ideally, such a classification scheme should be strongly underpinned by the basic functions of a catchment, such as mechanisms of water partitioning, storage, release and transmission within the catchment, potentially to be quantified by different catchment signatures, as suggested by Wagener *et al.* (2007).

A promising research avenue explored during the PUB Decade was the utility of catchment structure as a first step towards comprehensive classification schemes. One possible method is based on the assumption that the catchment structure should ideally be reflected in structures of catchment models (Fenicia *et al.* 2013). Identifying the most adequate model structure for a catchment from a suite of multiple competing model hypotheses (e.g. Clark *et al.* 2011a) can be seen as a robust first-order classification method, as demonstrated in a study involving around 200 catchments (Ye *et al.* 2012, Fig. 10). In an alternative approach, building on seminal work by Horton (1945), Strahler (1957) and Rodriguez-Iturbe and Rinaldo (1997) characterizing landscapes with the help of dimensionless numbers, Berne *et al.* (2005) were able to demonstrate the potential of dimensionless hillslope Peclet numbers to relate form, hydraulic properties and climate to hydrological response patterns. Lyon and Troch (2007, 2010) corroborated their conclusions by finding a good correspondence between analytically derived and observed moments of subsurface

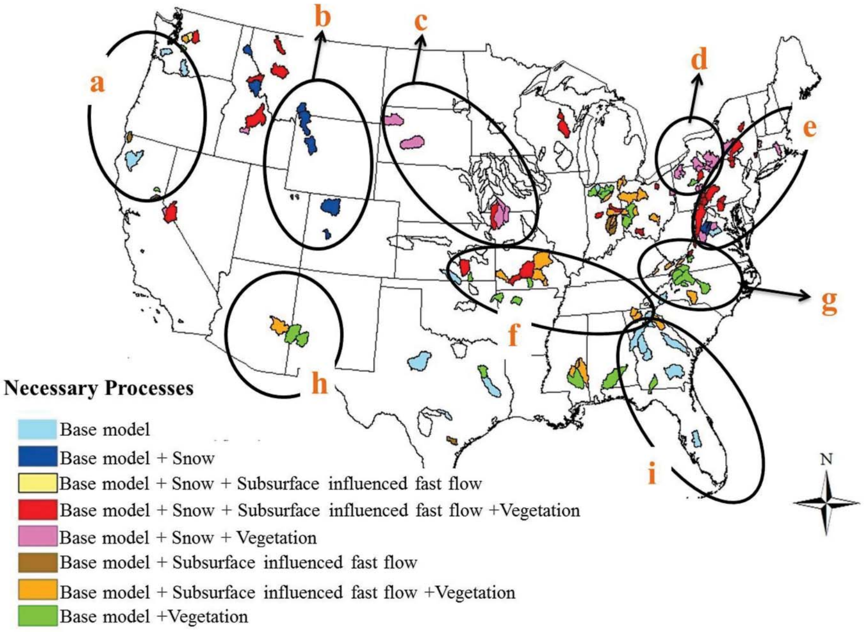


Fig. 10 Based on analysis of flow duration and regime curves, and the inferred influence of temperature, aridity, seasonality and phenology, the circled areas represent regions of process similarity. This indicates the need for models that represent the same dominant processes for catchments within the circled regions (from Ye *et al.* 2012)—an example of how careful synthesis of catchment emergent properties and signatures can guide the model design and selection process for data-scarce regions in particular.

response function as defined by hillslope Peclet numbers. Likewise, Harman and Sivapalan (2009) demonstrated a link between storage–release dynamics, boundary conditions and characteristic storage thickness. Including the concept of hydrological regimes, they argued that such a similarity framework can be used to classify hillslopes according to their subsurface flow dynamics.

In contrast, Woods (2003) developed models to predict differences between catchments based on dimensionless similarity parameters representing different aspects of topography, soil, vegetation and climate. Viglione *et al.* (2010) introduced similarity parameters for characterizing the space–time variability of flood processes. Accounting for the relative roles of network connectivity, hydraulic gradients and flow portioning between lateral and vertical flow paths within a given hydro-climatic region, Buttle (2006) introduced the T^3-template, a classification framework reflecting the relationships between portioning, transmission and release dynamic. However, as noted by Blöschl (2005), similarity measures differ in terms of the processes they aim to represent, and a reasonable choice of the measures depends on the understanding of the dominant runoff generation mechanism in both gauged and ungauged catchments. Kuchment and Gelfan (2009), for example, found that the dimensionless indexes derived from the Richards equation, i.e. Peclet number and capillary filtration efficiency, work well as similarity measures for the arid steppe region where the infiltration excess mechanism of runoff generation dominates.

Classification schemes based on hydro-climatic factors largely relate to the Budyko curve, plotting the catchment aridity index, i.e. the ratio of average annual potential evaporation over average annual precipitation, against the ratio of average annual actual evaporation over average annual precipitation (Budyko 1974). The Budyko curve thereby interprets the annual water balance as a manifestation of the competition between available water and available energy, as underlined by Sivapalan *et al.* (2011b). In spite of ambiguous interpretation possibilities (Andréassian and Perrin 2012), it can be seen as a simple tool for obtaining a first-order functional classification of catchments, as demonstrated, for example, by Tekleab *et al.* (2011). Building on the Budyko curve and extending the functional approaches of L'vovich (1979) and Ponce and Shetty (1995) to allow for analysis of regional and inter-annual variability in quick flow, slow flow and evaporation, Sivapalan *et al.* (2011b) were able to identify non-dimensional similarity metrics that can link regional to site-specific patterns, thus indicating a universal underlying relationship. Parajka *et al.* (2009b, 2010) pointed out the value of the seasonality of hydrological variables for inferring catchment similarity. Seasonality, along with catchment state and spatial coherence, was used by Merz and Blöschl (2003) to classify floods into types by their generating mechanisms such as synoptic floods, flash floods, snowmelt floods and rain-on-snow floods.

In a different approach, DiPrinzio *et al.* (2011) used self-organizing maps to classify around 300 catchments according to climate, structural and functional descriptors, while Sawicz *et al.* (2011), applying cluster analysis based on six functional signatures, such as the runoff coefficients and the slope of the flow duration curves, were able to classify around 300 catchments into nine clusters. Similarly, using four similarity metrics—the aridity index, the seasonality index, day of peak precipitation and day of peak runoff—it was shown that more than 300 catchments can be classified into only six classes (Coopersmith *et al.* 2012). In spite of within-class variability, this allows the determination of first-order differences in hydrological function between catchments. In an effort to synthesize the results of three of the studies discussed above (i.e. Cheng *et al.* 2012, Coopersmith *et al.* 2012, Ye *et al.* 2012), Yaeger *et al.* (2012) highlighted that climate seasonality and aridity were dominant controls on the regime curve of monthly mean flows, and were connected to the central slope of the flow duration curve. From that it could, in turn, be reasoned that the middle part of the flow duration curves, describing the average catchment response, is characterized by climate. In contrast, the low-flow ends of the flow duration curve were shown to be dominated by catchment characteristics, e.g. soils. This study illustrated the value of synthesis as structural and climatic controls, obtained from different approaches, could be combined to regionalize hydrological function (or model structures), thus marking a crucial step towards a unified classification framework.

3.3.3 Advances towards a new hydrological theory During the PUB Decade, an increasing understanding emerged that the hydrological system cannot be sufficiently well understood by focusing on the hydrograph alone (see Gupta *et al.* 2008). Given the importance of evaporative processes as the largest flux of both mass and energy in the system in many regions of the world, it was realized early that the dynamics and patterns of these processes need to undergo closer scrutiny (e.g. Brutsaert 1986, Gan and Burges 1990b, Grayson and Blöschl 2000). Therefore, a variety of studies started to more closely investigate evaporative processes, and to establish stronger links with our perception of the hydrological cycle at multiple scales from processes at the plant cell scale to organizational patterns at the global scale (e.g. Gerten *et al.* 2004, Savenije 2004, de Groen and Savenije 2006, Green *et al.* 2006, Siqueira *et al.* 2006, Teuling *et al.* 2006, Gerrits *et al.* 2009, 2010, Mahecha *et al.* 2010, Seneviratne *et al.* 2010, Van der Ent *et al.* 2010). For example, Thompson *et al.* (2011b) emphasized the combined roles of soils, temperature, as well as rainfall phase and seasonality, on seasonal dynamics of evaporation. Moreover, Troch *et al.* (2009b) were able to show, in a compelling study, that with decreasing water availability, water use of vegetation becomes more efficient and, independently from the boundary conditions, vegetation adapts to climate in similar ways. Similarly, the establishment of stronger links between hydrology, climate, vegetation and nutrient transport dynamics (e.g. Arnold *et al.* 1998, Dawson *et al.* 2002, 2008, Johnson *et al.* 2006, 2007, Abbaspour *et al.* 2007, Pacific *et al.* 2009) will be a promising way forward.

Results like these helped to acknowledge the importance of coupling hydrology, climate, soils and vegetation, and underpinned the need to widen our traditional concept of the water cycle to reflect a real systems approach. This was strongly emphasized by Kumar (2007), who argued that the property of the water cycle as a network of innumerable, self-organizing, dissipative feedback cycles must be more explicitly addressed. From there, it was only a small step to recognize the need to identify universal organizing principles, evolving from fundamental physical or biological laws, and to integrate the processes involved in the co-evolution of climate, soils, topography, vegetation and humans, ultimately leading the way to new, promising modelling strategies which could potentially include what were termed *behavioural modelling* approaches (Schaefli *et al.* 2011).

Following the co-evolution of the landscape with hydrology, vegetation—in a continuous feedback process—adapts to and shapes the hydrological system (e.g. Horton 1933, Savenije 2010). Thus, from a vast range of potential organizing principles (Paik and Kumar 2010), the set of ecological optimality hypotheses postulated by Eagleson (1978) is a promising candidate for a hydrologically meaningful organizational principle. Eagleson (1978) invoked three constraints on the state of vegetation, as discussed and reformulated by Sivapalan (2005): (a) over short time scales the vegetation canopy density is in equilibrium with climate and soil to minimize water stress of vegetation and to maximize equilibrium soil moisture; (b) over long time scales species will be selected whose transpiration efficiency maximizes equilibrium soil moisture equivalent to minimizing total evaporation; and (c) over very long time scales vegetation will alter soil properties and pore disconnectedness to maximize optimal canopy density. As underlined by Sivapalan (2005), possible combinations of climate–soil–vegetation systems can then be limited to relatively small subsets satisfying these three optimality constraints. In addition, the optimality approach could potentially facilitate predictions at any scale of interest, reducing the required model complexity and largely diminishing the need for calibration, thereby providing falsifiable models (Schymanski 2008). As an example, Schymanski *et al.* (2008, 2009) constrained plant transpiration, canopy cover pattern, CO_2 dynamics, root water uptake and rooting depth by maximizing net carbon profit, illustrating the effectiveness of optimality-based modelling when combining mechanistic approaches of water movement through the soil with evolutionary concepts accounting for plant functioning and adaption to the environment (Sivapalan 2009). As illustrated in Fig. 11, an optimality-based model could reproduce the main features of daily evapotranspiration rates and CO_2 assimilation observations, indicating that optimality may be a useful way of approaching prediction and estimation of vegetation cover, rooting depth and fluxes in ungauged basins without the need for calibration.

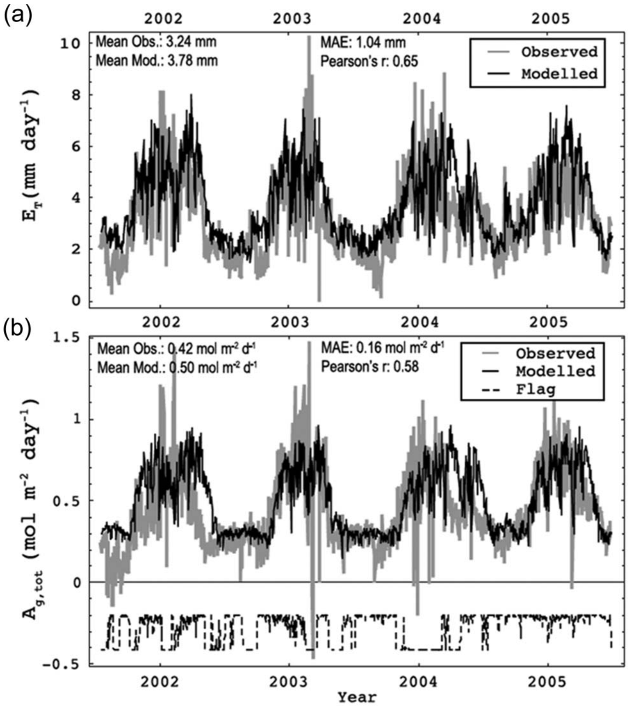


Fig. 11 Modelled (black) and observed (grey) daily (a) evapotranspiration rates (E_T) and (b) net CO_2 assimilation rates ($A_{g,tot}$). The means of the observed and modelled time series are given, together with the mean absolute errors (MAE) and Pearson's r values, indicating the goodness of fit (from Schymanski *et al.* 2009, © 2009 John Wiley and Sons, Ltd.).

Viewing hydrological systems as open, dissipative systems far from equilibrium and treating them in a thermodynamic framework offers new ways to explain catchment structure, formulate general constraints on their dynamics and their evolution in time (see Kleidon and Schymanksi 2008, Kleidon *et al.* 2010). Thermodynamics forms a common framework to describe stocks, fluxes, conversion and dissipation of energy. Apart from conservation of mass, it emphasizes conservation of energy (the first law of thermodynamics) and explains the direction of spontaneous processes from first principles (the second law of thermodynamics). Potential advantages of a thermodynamic approach are that (a) energy expressed as conjugate variables provides the link between energy and system states for any process, (b) by adding energy considerations in the centre of hydrological dynamics, additional system constraints based on additional observables can be formulated, (c) the second law provides a direction for system evolution, which deterministic physics does not, and (d) it allows one to formulate and evaluate general optimality hypotheses such as Maximum Entropy production (MEP): Wang and Bras (2011) proposed a model of evaporation over soils of variable wetness based on MEP; Porada *et al.* (2011) applied the same principle to estimate parameters related to root water uptake and runoff production in a global water balance model. The parameter values that maximize global entropy production also lead to reasonable reproduction of observed large river basin runoff. Schymanski *et al.* (2010) also applied MEP to predict the effect of heterogeneous vegetation cover on water fluxes and biomass. Zehe *et al.* (2010) applied the principle of Maximum Energy Dissipation to model preferential flow in soils, while Kleidon *et al.* (2013) investigated how systems with processes coupled by feedbacks evolve towards states of maximum power.

It is not yet entirely clear whether the optimality principle also applies at the time scales of the hydrological response and, if so, which optimality constraints apply, or how short-term changes of the system can be accommodated while at the same time making the most efficient use of available data. However, it may be seen that a careful synthesis of mechanistic or *Newtonian* approaches, describing how energy as well as mass fluxes defined by the boundary conditions of the system, and evolutionary or *Darwinian* approaches, characterizing patterns of variability (e.g. Kumar and Rudell 2010), has the potential, within the framework of comparative hydrology (Blöschl *et al.* 2013), to become valuable for achieving a deeper understanding of hydrological systems and of how they will evolve over time (Blöschl and Montanari 2010, Sivapalan *et al.* 2011a), possibly in the direction of a new holistic theory of hydrology.

4 HOW DID PUB EVOLVE OVER THE DECADE?

The PUB science plan (Sivapalan *et al.* 2003b) was the official document guiding the development of the PUB initiative and providing a starting point at the beginning of the PUB Decade. The initial science focus centred on the reduction of predictive uncertainty and evaluating the consequences of inadequate knowledge and its influence on uncertainty. Five broad community objectives for PUB were defined:

- to develop an extensive observational field programme in research watersheds across the world;
- to increase awareness of the value of data and the need for targeted gauging of currently inadequate data sources;
- to advance capability to make predictions in ungauged basins based on local knowledge;
- to advance the understanding of the links between climate, landscape and hydrological processes; and
- to promote capacity building.

These objectives, centred around the quest to reduce predictive uncertainty, were to be addressed by six specific PUB science questions:

1. What are the gaps of knowledge?
2. What are the requirements to reduce uncertainty?
3. What experimentation is needed?
4. How can observational technologies be used to improve predictions?
5. How can process descriptions be improved to reduce uncertainty? and
6. How can the value of data be maximized?

The science questions were investigated from different perspectives, as highlighted by the six parallel science themes (see Section 2), in an attempt to reach the actual targets of PUB, i.e. improving existing and developing new models based on improved process understanding with reduced need for calibration, which were conceived to be the necessary steps forward at that time. The way scientific understanding evolved and thinking shifted towards new questions during the PUB Decade is sketched in Fig. 12 and outlined briefly below.

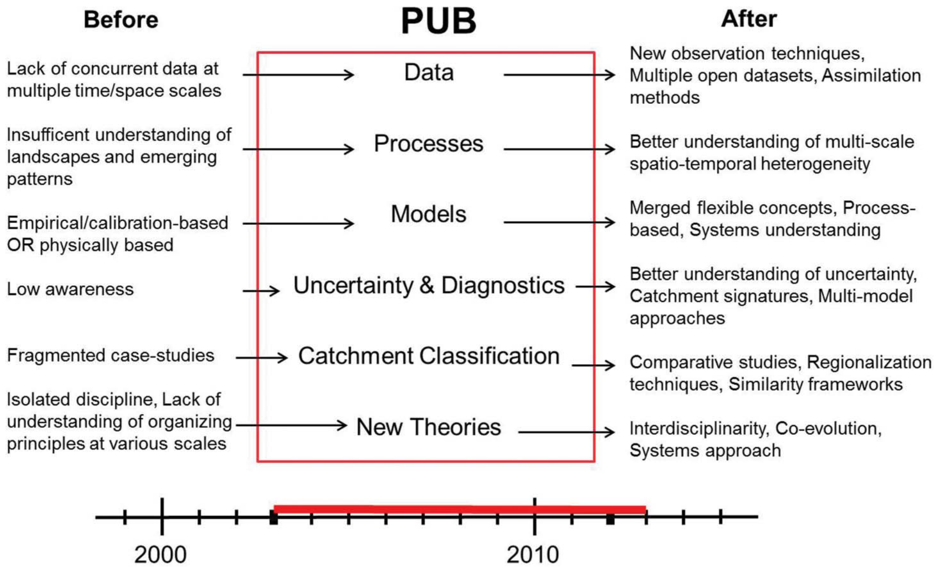


Fig. 12 Outline of how scientific understanding evolved and the way of thinking shifted towards new questions during the PUB Decade.

Within the context of PUB, the emphasis on data was seen as offering the opportunity to develop a better understanding of patterns and dynamics of the underlying processes in both gauged and ungauged catchments in order to pursue the goal of reducing the predictive uncertainty in these catchments. Besides advances in observation technology (see Sections 3.1.1 and 3.1.2), considerable efforts were thus made to ensure the availability of a wide spectrum of hydrological and water quality data from existing or new experimental catchments (see Sections 3.1.3–3.1.5). In spite of sometimes considerable uncertainties associated with data, a major stepping stone towards an improved understanding and characterization of process heterogeneity was the understanding of the value of pooling data from catchments in contrasting environmental settings for comparative studies, thus explicitly investigating the links between process heterogeneity and climate, vegetation and geology. Data analysis also allowed the evaluation of different types of data, thus feeding back into data acquisition by guiding targeted future observations necessary for an improved understanding.

It was gradually realized that many existing model concepts, although sometimes applied out of context, were not unreasonable representations of the dominant processes underlying the catchment response. This is reflected in the continued use of many "old" models and only a limited number of significantly different, new model formulations (see Sections 3.2.1 and 3.3.3). However, important progress was made in actually better understanding these models and the interactions between their parameters. This led to more targeted applications of different models at different locations, and endorsed the use of explicitly flexible modelling strategies to better accommodate the varying importance of different processes in different locations, while at the same time maintaining the goal of model parsimony. In a further development, both pooled data and advances in model diagnostic methods (see Section 3.2.2) resulted in a better founded appreciation and understanding of different sources of uncertainty and the resulting implications. Not only was the need to disentangle data, models and parameter uncertainty strongly underlined in order to allow a more adequate treatment of these different aspects of uncertainty, but a lively discussion developed as to whether it is actually possible to largely eliminate uncertainty in models as was originally hoped for (see Section 3.2.4). It was increasingly realized that in the presence of considerable uncertainties in data, i.e. models are forced with erroneous input and calibrated to erroneous output data, it is almost impossible to unambiguously identify the most suitable model(-parameterization) for a given catchment, whose boundary conditions are, in addition, largely unknown. Further, systems characterized by organized complexity can be subject to considerable system intrinsic uncertainty. This is related to threshold processes and their feedback mechanisms and can reduce the predictability of a system that is in principle deterministic. However, the importance of these effects is subject to an ongoing debate. Intimately linked to the problem of uncertainty, and at the core of PUB, is the question whether hydrology can reduce the need for calibration. Besides the importance and efficiency of calibration for data-driven modelling approaches (see Section 3.2.1), an understanding developed that, in the presence of the above uncertainties, a better understanding of the system alone, although an important premise, may not necessarily result in reduced predictive uncertainty, and that a certain level of calibration may frequently be unavoidable. However, a number of studies demonstrated the potential of "soft" data, emergent properties or expert knowledge to, partly *a priori*, constrain predictive uncertainties. This, in turn, may limit the need for calibration, thereby highlighting the importance of this research avenue for actually improving predictions in ungauged basins (see Section 3.2.5). These critical points resulted in some additional priorities for PUB, including the quest for a better understanding of uncertainties, both in the system and in data, possible ways to characterize them and calls for innovations in observation technologies to reduce data errors, all of which were to be understood as additional means towards improved understanding of catchment functioning.

In a constant feedback process, data from comparative studies together with results from modelling studies resulted in considerable steps forward being made in linking catchment form to catchment function. This resulted in some success in the development of catchment classification schemes, similarity frameworks and model regionalization methods for transferring knowledge and improving predictions in ungauged basins (see Sections 3.3.1 and 3.3.2), although the further potential of these methods might at present be limited by data uncertainty. The better links between catchment form and function also led to the understanding that seeing hydrology as an integral part of the ecosystem may not only create a better understanding of organizing principles, but could also direct the way towards alternative, holistic modelling strategies, some of which are currently being explored for feasibility and utility (see Section 3.3.3).

A critical objective of PUB was also to promote capacity building and to improve knowledge transfer to operational hydrologists. Although difficult to assess objectively, it can be said that the success was variable, largely depending on individual countries and the degree to which communication between researchers and practitioners was actively fostered by local stakeholders. One of the main reasons knowledge transfer was sometimes incomplete could be the frequently strong focus on what may be perceived as theoretical issues or relatively complex methods. Temporal constraints, but also sometimes contrasting ways of thinking in engineering hydrology, make it difficult to fully appreciate academic advances in the field. It thus seems that capacity building needs a stronger and clearer community outreach, possibly in the form of workshops, such as the "Putting PUB into Practice" workshop (Pomeroy *et al.* 2013), or publications dedicated to hydrological practice, addressing new advances from the perspective of practitioners, as illustrated in the Case Study Section of Blöschl *et al.* (2013).

Although it is certainly too early for a final assessment, and the effect of some contributions will only became visible in the future, it can be stated that the PUB initiative reached some of its initial goals, while other objectives remained elusive or too ambitious for the given time frame. The major achievement of PUB is probably its openness and flexibility in the shifting of critical objectives and the formulation of new relevant questions, addressing issues which were unknown at the beginning of the PUB Decade and which arose from the results of pursuing the original PUB targets.

5 IMPACT OF PUB ON THE HYDROLOGY COMMUNITY AND THE ROLE OF IAHS

In addition to considerable scientific advances during the past decade, as summarized in the sections above, the PUB initiative, under the organizing umbrella of the IAHS, played an important role in shaping the ways in which the hydrology community works together. It is clear that PUB did, in fact, act as an efficient unifier and catalyst, even if not all papers discussed above explicitly refer to PUB. It was instrumental in bringing the global hydrology community closer together, thereby establishing a much needed culture of inclusivity, promoting openness and an increasing sense of community. This helped to develop a common language between different research groups with different research foci worldwide. In addition, PUB provided common purpose to scientists from diverse parts of the hydrology community, such as systems theorists, modellers, experimentalists and theoreticians, by guiding the definition of clear core questions of where progress is needed to advance hydrology as a science, as illustrated by Fig. 13, summarizing the relevance of different aspects and concepts in hydrology throughout the PUB Decade. All these efforts contributed to energize the community and to increase collaboration and interdiciplinarity among individual research groups. The result was an accentuation and encouragement of explicit knowledge building through *comparative hydrology*, rather than by mere knowledge accumulation, and facilitated the first steps towards

Fig. 13 Word cloud summarizing the relevant aspects and concepts of hydrology throughout the PUB Decade, based on the index of Böschl *et al.* (2013).

hydrological synthesis across processes, places and scales (Blöschl *et al.* 2013).

Arguably a primary reason for the success of the PUB initiative was its conception and execution as a grass-roots (bottom-up) movement. The leadership deserves credit for actively encouraging and empowering the self-organization of PUB "working groups", which ultimately investigated a very wide range of topics that could not have been conceived of by a top-down approach. Further, as PUB was neither a funding organization, nor as an organization itself received significant funding, scientists and research groups naturally felt the need and benefit of closer collaboration to share data and knowledge, thus turning a "negative into a positive" and achieving much of the progress *because* of no available funding rather than *in spite* of it (participants needing funding instead actively exerted pressure on other sources, such as national funding agencies). This resulted in the development of a consensus that hydrology benefits from being a "team science", and that progress is not just about the science, but is also about enabling the people to channel their self-interest towards the common interest.

Of course, IAHS provided the organizational framework for PUB and, by granting access to its infrastructure, played a significant role in the community building process. The global outreach of IAHS contributed to the crucial objective of inclusivity. In particular, IAHS offered a platform and adequate infrastructure to enhance and coordinate a wide variety of PUB-related working groups, such as the Working Group on Uncertainty Analysis in Hydrologic Modeling (WG-UAHM, Meixner *et al.* 2004) and many more named in Franks *et al.* (2005). Furthermore, numerous PUB-related workshops were organized, e.g. the Swedish IHP nutrient-model comparison workshop (2011) and the Canadian Water Resources Association's "Hydrology for the orographically challenged" PUB workshop (2005). The "Putting PUB into Practice" Workshop in 2011 was attended by PUB hydrological scientists and practitioners from every inhabited continent, and contributed to the transfer of improved prediction techniques to hydrological practitioners and the identification of problems in established techniques, the solution of which PUB could contribute to (Moore *et al.* 2013, Pomeroy *et al.* 2013). This workshop was meant to address a pressing need to outreach the progress made during the first three PUB biennia to the practicing hydrology community. Besides workshops, PUB-related sessions at major conferences were organized, e.g. at the IAHS general assemblies in Foz d'Iguasso (2005), Perugia (2007), Hyderabad (2009) and Melborne (2011), as well as at the annual European Geosciences Union (EGU) general assemblies and the American Geophysical Union (AGU) fall meetings. In addition, a range of PUB-related IAHS Red Books (de Boer *et al.* 2003, Franks *et al.* 2005, Schertzer *et al.* 2007, Xu *et al.* 2008, Yilmaz *et al.* 2009), and all articles therein, have acted as periodic catalysts during the decade, while other thematic and IAHS commissions' Red Books during the decade have cross-cut and fed many of the issues reviewed above (e.g. Tchiguirinskaia *et al.* 2004, Oki *et al.* 2006, Boegh *et al.* 2007, Webb and de Boer 2007, Refsgaard *et al.* 2008, Hermann *et al.* 2010, Khan *et al.* 2010, Oswald *et al.* 2012). Several PUB-related papers have been distinguished, such as the Tison Awards for the papers by Cudennec *et al.* (2006), Laaha and Blöschl (2007), Valery *et al.* (2009) and Love *et al.* (2010). This highlights the active and important role of IAHS throughout the PUB Decade, until the closure at the Delft conference, the PUB synthesis book (Blöschl *et al.* 2013) and this review paper. The entire community process is capitalized through the PUB page at www.iahs.info, including the podcast of the Delft conference plenaries.

In general, the PUB initiative has provided a model for how community activities should be carried out to ensure scientific progress across a discipline, with the important concepts of *grassroots*, *empowerment* and *plurality* being the cornerstones of success and dynamic development.

6 WHAT ARE THE CHALLENGES AND OPPORTUNITIES AHEAD?

The PUB Decade saw considerable progress in the development of hydrology as a science. However, given that the Earth is in the Anthropocene era (e.g. Crutzen and Steffen 2003), characterized by on-going change and increased human impact on the water cycle, much effort is still required to better understand, model and especially predict the dynamics of the system (Wagener *et al.* 2010), which in turn is also partly dependent on our ability to characterize and understand uncertainty in the data available.

On the one hand, while acknowledging data as the backbone of scientific understanding, the dialogue between experimentalists, modellers and theoreticians needs to be strengthened to ensure that critical data are both collected and shared. This relates not just to improved data quality and quantity of variables such as precipitation, flow or evaporation, but clearly also extends to new types of data and underexploited data from fields outside hydrology, such as ecology or sociology, which can help to integrate and synthesize our knowledge of hydrological response patterns. A considerable challenge, hereby, will be to develop a better understanding of the value of different kinds of data and their possible uses. This also includes necessary advances in assimilating potentially contradicting sources of information. A further critical need is more effective pooling of data, i.e. "large sample hydrology" (e.g. Andreassian *et al.* 2006, Gupta *et al.* 2013), and that we understand and try to benchmark the quality and errors in our data by sharing such knowledge (see McMillan *et al.* 2012b). In the comparative hydrology approach, large data sets can then be used to learn from the similarities and differences between catchments in different places, and to interpret these in terms of underlying climate–landscape–human controls (Blöschl *et al.* 2013).

There is already increasing consensus in the community that data need to be more easily accessible. Developing new strategies to promote data sharing, designing global open access databases, such as the *EVOp* (www.evo-uk.org) and *Earthcube* (earthcube.ning.com) projects currently under development, and similar to what is sometimes already available on a national basis (e.g. France, USA or Sweden), as well as devising standardized data storage formats and protocols, as pursued for example by the *Open Geospatial Consortium* (www.opengeospatial.org), is thus paramount, while also giving adequate credit to the experimentalists who invested considerable effort, time and money in the generation of these data sets. In addition to finding a data-sharing consensus within the scientific community, policy and decision makers need to be more closely involved in the discussion process to facilitate easier access to government data and to ensure continuous funding of baseline data collection, such as discharge and precipitation. Open data policies will then inevitably raise questions of where these data should best be stored, who will be responsible for data management, quality control, documentation (i.e. metadata) and maintainance, how data management will be funded, or how the increasing amounts of data should best be handled. Open data policies and virtual laboratories could ideally also be extended to encourage the community to make source codes, including detailed documentation, openly available through source code libraries, possibly featuring discussion forums, which can facilitate transparent model improvement by knowledge exchange. Furthermore, the community could strongly benefit from the increased use of online information repositories, such as the Experimental Hydrology Wiki (www.experimental-hydrology.net), or the Catchment Change Management Hub (www.ccmhub.net). Tightly linked to the idea of discussion forums and online information repositories is the need for improved community outreach, as not enough of the advances made during the PUB Decade actually found their way into engineering hydrology, thus limiting the impact the new science had in practice. Hydrology as a science will also benefit from a generally more inter-disciplinary strategy, with inter-disciplinary education and joint inter-disciplinary research efforts in designated research catchments, as well as special emphasis on site inter-comparison studies (Blöschl *et al.* 2012).

Another opportunity for the hydrological community is to engage in recently completed artificial hillslope research infrastructure, such as the Landscape Evolution Observatory (LEO; e.g. Hopp *et al.* 2009) in Arizona, USA, Hydrohill in China (Kendall *et al.* 2001), or Chicken Creek in Germany (Holländer *et al.* 2009). These research facilities offer the opportunity to conduct controlled experimentation under various environmental conditions (artificial rainfall in Hydrohill and fully controlled environmental conditions in LEO) to address critical questions, such as subsurface network flow and structural development and hillslope threshold behaviour. These densely instrumented research facilities will generate extremely valuable hydrological and geochemical data sets that can be used by the hydrological community for hypotheses testing regarding flow processes, as well as for model intercomparison and development. In addition, the scientists that manage these facilities are open to interaction and iterative design of specific experiments (e.g. Huxman *et al.* 2008).

However, considerable challenges still clutter the way towards improving modelling and uncertainty assessment strategies. In fact, there is still a long way to go in terms of predictions: much of the success so far has been in gauged and not in ungauged basins. This is particularly problematic for developing countries, as they are most affected by the inability to make more reliable predictions, thereby limiting the ability to efficiently manage their water resources and to mitigate the effects of floods and droughts. In addition, no consistent harmonization of modelling strategies has been achieved so far. A significant challenge is in developing modelling approaches that incorporate multi-scale nonlinearities to permit process up-scaling and to account for emergent processes from the grid-cell to the catchment scale. Also, ways need to be sought to improve *a priori* accumulation of theoretical information for parameter and model structure identification in order to limit calibration requirements and the importance of equifinality. Moreover, the modelling community needs to devise more stringent and standardized test procedures to select the best model formulation out of a variety of competing model hypotheses for a given stated application. Further, it will be important to strengthen data and model diagnostic tests to more efficiently extract information on model deficiencies, including error structure and dynamics (Gupta *et al.* 2012). This can then lead the way, not only to a better understanding of spatio-temporal information transferability, but also to detect non-stationarities, due to epistemic error in data or natural fluctuations of, as well as human influence on, the system, and to develop methods of incorporating them in models. Another crucial aspect to be addressed will be the development of a universal uncertainty assessment framework that permits evaluation of uncertainty in line with probability theory, while ensuring explicit and combined treatment of different error types and non-stationarity in error structures. This will require not only a separation of data and model errors, but also the definition and identification of (dis)information in data, thereby moving towards a separation of epistemic and aleatory errors. If future developments in observation technology manage to reduce epistemic errors, in particular as a result of higher spatio-temporal resolution and measurement precision, and if patterns in the non-stationarity of these errors can be characterized, such efforts could ultimately lead to the definition of non-stationary, formal likelihoods that explicitly reflect these different types of error.

Adequately addressing the challenge of ungauged basins, especially in the light of change, will thus require the development of a better understanding of how hydrological function links to catchment form. Comparative hydrology may hold one of the keys to synthesizing the knowledge of interlinked nonlinear processes across space and time scales on the way towards a unified hydrological theory. Furthermore, model strategies will eventually have to embrace the importance of feedback loops in the system and potential organizational principles, underlying the hydrological response. A critical step towards the identification and understanding of such organizing principles will be the detection of nonlinearities in the system and the development of a better understanding of threshold processes underlying these nonlinearities, with particular focus on their mutual interactions. Successful process regionalization and the design of universal catchment classification frameworks will largely depend on our ability to reconcile climate, form (including human influence on the system) and function. In other words, an enhanced understanding needs to be developed on what constitutes catchment function, or which boundary conditions are necessary for a certain catchment function to emerge; thus: What are the root causes of hydrological similarity? Together with an improved understanding of threshold patterns, the establishment of robust links between climate, form and function will be instrumental in the quest for overarching organizational principles controlling the hydrological response at any scale—the foundation of a universal hydrological theory.

7 CONCLUSIONS

The PUB initiative set out to develop a better scientific basis for hydrology, permitting the development of more realistic models and thereby reducing prediction uncertainties. A decade of world-wide research efforts has resulted in considerable advances for hydrology as a science. While the PUB synthesis book (Blöschl *et al.* 2013) organizes the findings of the PUB Decade from the perspective of predicting runoff signatures, this paper has reported on the achievements of the PUB Decade from the perspective of the six PUB science themes.

Clearly, the PUB initiative was highly productive, as reflected in the literature review of this paper and the number of scientific publications that have cited PUB-related work. At the core of the scientific progress were the following achievements:

1. The development of an improved understanding of the ensemble of processes underlying the basin rainfall–runoff and snowmelt–runoff responses, and increasing consensus on the importance of thresholds, feedback processes and organizing principles that emerge from them.
2. The advances in process understanding have been key for developing a better understanding

of our models together with the associated uncertainties. This, in turn, facilitated the design of new modelling and uncertainty assessment strategies, and paved the way for identifying and addressing the challenges that lie ahead—challenges that relate to understanding the connection between catchment form and function, i.e. for strengthening the link between understanding our models and understanding our catchments, and the still-needed identification of suitable organization principles underlying the catchment response.

3. A relatively broad awareness emerged during the PUB Decade that flexible approaches to modelling, that allow the adjustment of models to specific environmental conditions in different catchments, and model falsification, can be highly beneficial, as the stronger focus on site-specific dominant processes has shown to have the potential to reduce predictive uncertainty.
4. The potential of models as tools for learning about catchment function is now widely recognized and explored.
5. It is now commonly accepted that hydrology needs systematic and consistent uncertainty assessment, acknowledging and quantifying different sources of uncertainty as well as different types of errors, although no consensus has been reached as to how this is best done.
6. The need for and benefits of comparative hydrology to gain a better understanding of emergent processes, eventually leading to the understanding of organizational principles underlying the catchment response, were recognized, making comparative hydrology an important tool that has made its way into mainstream hydrology.
7. The improved understanding of the links between catchment form and function, often based on emergent properties, i.e. catchment signatures, led to the first promising steps towards functional catchment classification.
8. From a synthesis of data, process understanding and the link between catchment form and function, possible ways towards identifying organizing principles and an eventual formulation of a unified theory were outlined, based on a combination of *Newtonian* and *Darwinian* approaches.

Apart from scientific advances, significant achievements were made in community building, which will be instrumental for ensuring future progress in the discipline. In particular, the PUB initiative has:

9. brought the global hydrology community closer in terms of communication and collaboration, thus gradually replacing mere information accumulation with new knowledge generation;
10. unified the field around core questions and provided a common purpose to modellers, experimentalists, theoreticians, etc.;
11. helped to create a common language between different research groups with different research foci, thus facilitating more collaboration; and
12. provided a model for what community activities should be based on: grassroots, inclusivity, empowerment and plurality.

However, some challenges remain to be addressed:

13. There is still a long way to go in terms of achieving robust and reliable predictions: much of the success so far has been in gauged rather than in ungauged basins, which has negative effects in particular for developing countries, where inabilities to make reliable predictions will continue to impede sustainable water resources management and the development of effective flood and drought mitigation strategies.
14. The progress made in the PUB Decade has not led to the harmonization of modelling strategies that was hoped for.
15. Although there has been significant activity in transferring PUB findings into practice and the political decision-making process (see e.g. Savenije and Sivapalan 2013), more efforts are needed to ensure sustainable water resources management strategies.

These challenges must be addressed, especially in the context of variability resulting from both naturally occurring and anthropogenically triggered fluctuations of the system. Underpinning and emphasizing the importance of change has naturally led to the new hydrological science initiative for the upcoming decade being called Panta Rhei—Everything Flows (Montanari *et al.* 2013).

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Symposium 2012—a mere subset of the large number of scientists who contributed to the overall progress made. The enthusiasm and active participation of the world-wide hydrological community towards advancing science through ideas, comments and constructive criticism have been extremely valuable. In compiling this review, the authors have tried to be inclusive, but may have overlooked and missed some important work. The authors are especially grateful for the critical and constructive comments on an earlier version of the manuscript submitted to *HSJ* that were received from Keith Beven, Andreas Efstratiadis, Demetris Koutsoyiannis, Ioannis Nalbantis, Kuni Takeuchi and one anonymous reviewer, which helped in making substantial improvements to the content and presentation of the paper. Further, the support of Susan Steele-Dunne for sketching out the advances in observation technology is greatly acknowledged. Finally, the authors especially acknowledge the contribution of Gaelle Hrachowitz-Fourcade for drafting a French-language abstract for this manuscript. Two authors of this paper, Markus Hrachowitz and Doerthe Tetzlaff, would like to use this opportunity to pay tribute to Julian J. C. Dawson, an inspirational scientist, (co-)author of several PUB-relevant publications, as well as a former colleague and good friend, who died in a car accident during the preparation of this manuscript.

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