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Key Points:

- Recent breakthroughs in fields such as geostatistics, analytical chemistry, remote sensing, or data assimilation are discussed
- The relevance of these emerging approaches in characterizing streambeds and modeling river-groundwater interactions is reviewed
- Integrating approaches across a range of spatial and temporal scales moves our current conceptual models toward the complexity of natural systems

Correspondence to:
P. Brunner,
philip.brunner@unine.ch

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Advances in understanding river-groundwater interactions

Philip Brunner[1], René Therrien[2], Philippe Renard[1], Craig T. Simmons[3], and Harrie-Jan Hendricks Franssen[4]

[1]Centre of Hydrogeology and Geothermics, Neuchâtel, Switzerland, [2]Département de géologie et de génie géologique, Université Laval, Quebec, Quebec, Canada, [3]National Centre for Groundwater Research and Training and School of the Environment, Flinders University, Adelaide, South Australia, Australia, [4]Agrosphere (IBG-3), Forschungszentrum Juelich GmbH, Jülich, Germany

Abstract River-groundwater interactions are at the core of a wide range of major contemporary challenges, including the provision of high-quality drinking water in sufficient quantities, the loss of biodiversity in river ecosystems, or the management of environmental flow regimes. This paper reviews state of the art approaches in characterizing and modeling river and groundwater interactions. Our review covers a wide range of approaches, including remote sensing to characterize the streambed, emerging methods to measure exchange fluxes between rivers and groundwater, and developments in several disciplines relevant to the river-groundwater interface. We discuss approaches for automated calibration, and real-time modeling, which improve the simulation and understanding of river-groundwater interactions. Although the integration of these various approaches and disciplines is advancing, major research gaps remain to be filled to allow more complete and quantitative integration across disciplines. New possibilities for generating realistic distributions of streambed properties, in combination with more data and novel data types, have great potential to improve our understanding and predictive capabilities for river-groundwater systems, especially in combination with the integrated simulation of the river and groundwater flow as well as calibration methods. Understanding the implications of different data types and resolution, the development of highly instrumented field sites, ongoing model development, and the ultimate integration of models and data are important future research areas. These developments are required to expand our current understanding to do justice to the complexity of natural systems.

1. Introduction

Streams and rivers are a major component of the water cycle, and they also shape landscapes, transport mass, and energy and provide ecosystem services. As a result, they have been studied by scientists from a wide range of disciplines, including hydrogeology and hydrology [*Sophocleous*, 2002], biology and ecology [*Boulton and Hancock*, 2006; *Hancock et al.*, 2005], geomorphology [*Lane et al.*, 2003; *Poole*, 2010], sedimentology [*Packman and MacKay*, 2003; *Rosenberry and Pitlick*, 2009a], and chemistry [*Dahm et al.*, 1998]. The approaches and methods employed in these disciplines differ, and it is therefore not surprising that vastly different perspectives, as well as methodological approaches, have evolved. Moreover, the spatial scales analyzed span many orders of magnitude (see Figure 1). The "hyporheic scale" (1–100 m) describes the spatial scale of the transition zone where hyporheic flow occurs (as indicated in the close-up figure on the right). The "reach scale" (100 to more than 1000 m) refers to the spatial scale dominated by the ambient groundwater conditions. The "catchment scale" (typically greater than kilometers) refers to even larger scales and corresponds to the whole catchment in which regional flow occurs. The numbers provided serve as an indication only. There is no universally accepted quantitative definition of these spatial scales.

However, despite all of these different scales and perspectives, a common denominator in the different disciplines is the streambed. The streambed constitutes the interface between the river and groundwater, and it controls river-groundwater interactions. It also consists of contrasting physical, chemical, and biological environments. While current water management tends to use efficient yet simplified models, there is a trend toward using integrated surface and subsurface hydrological models (ISSHMs) for managing water resources at the catchment scale. These approaches rely on improved conceptualization and characterization of the streambed [*Paniconi and Putti*, 2015].

A range of review and research articles have focused on the physical, chemical, and biological processes as well as the physical properties in streambeds [e.g., *Boano et al.*, 2014, *Constantz*, 2016]. These studies have

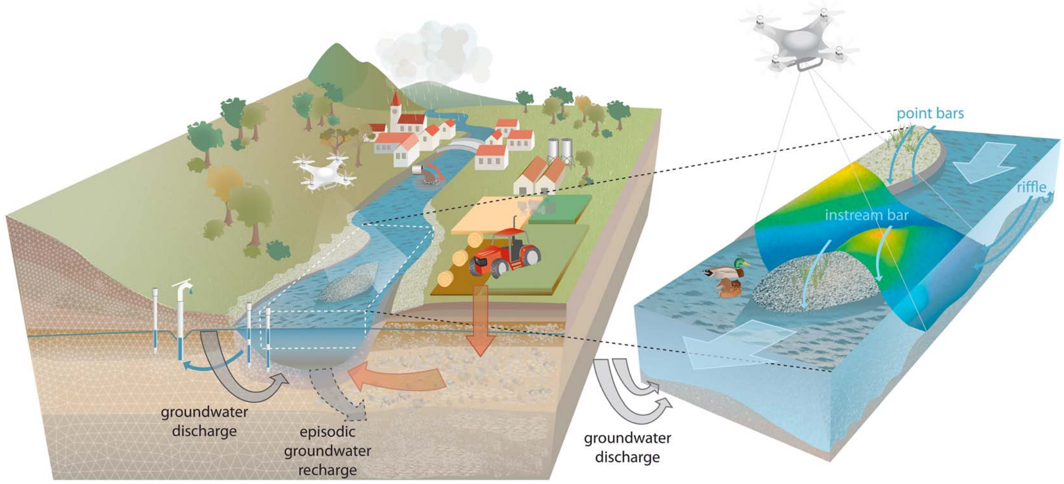

Figure 1. Schematic representation of an anthropogenically modified catchment. The interaction between groundwater and surface water creates numerous challenges related to water quality, quantity, and ecology. The figure illustrates the nested spatial scales of river water and groundwater interactions. (left) The reach scale is illustrated. (right) Hyporheic scale is shown. The technological advances and modeling approaches discussed in this paper provide information across a wide range of scales, and are aimed at a better characterization of the surface (e.g., through drones), the subsurface (e.g., hydraulic observations of water table dynamics or hydraulic properties of the streambed and its conceptualization in numerical flow models), and at measuring exchange fluxes between the surface and the subsurface.

uncovered numerous interactions and feedback mechanisms between hydraulic, sedimentological, biotic, and chemical processes in the streambed. For example, the deposition of fine sediments can lead to the reduction (streambed clogging or colmation) of the hydraulic conductivity of the streambeds [*Schalchli*, 1992] which affect river-groundwater interactions. The growth of biofilms also reduces the hydraulic conductivity of the streambed [*Battin and Sengschmitt*, 1999; *Ulrich et al.*, 2015]. Apart from biofilm growth, other biological processes can give rise to complex physical interactions and feedback mechanisms in streambeds. *Song et al.* [2007], for example, observed high values of hydraulic conductivities in the shallow streambed and associated these findings with increased invertebrate activities. The importance of a holistic consideration of hydrology, hydrogeology, sedimentology, and ecology is increasingly being recognized in various contexts, e.g., in the context of streambed habitats [*Stubbington*, 2012; *Groll et al.*, 2016], river restoration [*Beechie et al.*, 2010], and the transport and fate of contaminants [*Boano et al.*, 2014].

The scientific analysis of river-groundwater interactions across all relevant spatial scales is critical for solving a wide range of contemporary challenges that are illustrated with a few examples in Figure 1. Water quality issues arise from point sources such as a water treatment plant or diffuse sources such as the widespread application of pesticides [*Lapworth et al.*, 2012]. In both cases, the contamination will follow the river-groundwater interactions and affect both groundwater and streams [*Meals et al.*, 2010]. Groundwater abstraction near rivers or the diversion of river water can reduce streamflow, with critical consequences for ecological systems [*Poff and Zimmerman*, 2010]. Modifications to the stream (e.g., through channelizing rivers or instead revitalizing them) can significantly influence river-groundwater interactions by, for example, reducing hyporheic exchange [*Boano et al.*, 2014].

As the streambed is the controlling interface between surface water and groundwater, one would expect that simulations of the exchanges and interactions reflect these complexities and that the means for assessing uncertainties related to model simplifications are developed. In fact, significant research efforts have recently increased toward the development of spatially distributed hydrologic models that fully integrate surface and subsurface water flow. Distributed in this context means that parameters are spatially and temporally distributed, rather than a lumped system model where the hydrologic system is treated as a black box. *Paniconi and Putti* [2015] provided a detailed review of those integrated surface and subsurface hydrological models which are based on the blueprint presented by *Freeze and Harlan* [1969] for a physically based hydrologic response model (see Tutorial 1). On a conceptual basis, physically based models have widely been used to understand the basic physics of between rivers and aquifers [*Banks et al.*, 2011; *Brunner et al.*, 2009; *Doble et al.*, 2012;

Shanafield et al., 2012; *Xie et al.*, 2014] and have assisted in assessing the reliability of field methods [*McCallum et al.*, 2010; *Su et al.*, 2016]. Based on the original Freeze and Harlan blueprint, *Partington et al.* [2017] proposed an updated blueprint for a model capable of simulating the interactions and feedback mechanisms between hydraulic and sedimentological processes. Further extensions of the original blueprint that could, for example, integrate biological processes are possible.

However, despite these recent advances in the field of numerical models, current modeling practice is still far away from incorporating the full complexity of surface water and groundwater interactions. The current conceptualization of streambeds in numerical models that simulate surface water and groundwater interactions is greatly simplified at all relevant spatial scales. Streambeds are routinely simulated as static, homogeneous entities [*Partington et al.*, 2017; *Irvine et al.*, 2012]. Moreover, the types, quantities, and the quality of observation data used in the conceptualization and calibration of numerical models are typically limited to a small number of observed river stage levels and hydraulic heads in adjacent aquifers or river discharge rates. The simplified conceptualization of complex surface water-groundwater interactions creates major uncertainties that potentially remain undiscovered given limited field observations that are used in the modeling process. Other unresolved issues in current modeling practice are the appropriate level of complexity to incorporate in a model regarding processes, scale, and heterogeneity.

There have been, however, dramatic improvements in a variety of scientific disciplines that have not yet found their way into ISSHM. The focus of this review is integrated hydrological modeling and hydraulic characterization of alluvial river-groundwater systems. The main contribution of this paper is a review of advances in measurement techniques, geostatistics, and inverse methods and the new possibilities and applications that might allow an improved characterization of the streambed and river-groundwater interactions. We also consider methods that may not appear to be directly related to ISSHM at first glance but have the potential to lead to model improvements (e.g., the development of a miniaturized gas chromatographer, medical tomography, or cloud computing). We finally provide a subjective prognosis for this field of research and describe the current challenges and future opportunities.

This review paper describes methodological advances focused on river-groundwater interactions across the streambed and within the main channel. We acknowledge that in many rivers, substantial hydrological exchange occurs in the riparian zone and alluvial floodplains with coarse sediments. While we do not focus explicitly on advances that specifically pertain to broader interactions across riparian zones and floodplains, we anticipate that the methods discussed in this paper are likely to be broadly applicable to those environments.

2. Advances in Characterizing the Physical Environment of River-Aquifer Systems

2.1. Approaches to Characterize the Geological and Morphological Properties of Streams

2.1.1. Hydraulic Conductivity of the Streambed: From Point Observations to 3-D Structures

Hydraulic conductivity K ($L\,T^{-1}$), with L representing length and T representing time, is the ratio of water flow velocity to hydraulic gradient [*Fetter*, 2001]. It is a measure of the ease or ability of a fluid to flow through a porous medium and is a function of the properties of the porous medium (solid matrix) and the fluid flowing within it. It is therefore a lumped parameter that integrates the permeability of a porous medium with the fluid viscosity and density. High values are found in coarse sediments such as sand and gravel, while finer materials, such as silt and clay, exhibit low values. Heterogeneity of the hydraulic conductivity in the streambed has been identified as a crucial issue for hyporheic zone research [*Boano et al.*, 2010] as well as riparian zone and floodplain dynamics [*Camporeale et al.*, 2013].

Hydraulic conductivity is an important parameter relevant to essentially all fields of surface water and groundwater interactions, including ecological, biogeochemical, and hydraulic processes in the hyporheic zone [*Boano et al.*, 2014]. Hydraulic conductivity also controls large-scale exchange fluxes across the streambed (e.g., reach scale or catchment scale) and is thus required in the estimation of exchange fluxes with hydraulic methods (see section 2.3.2). Streambeds are likely to exhibit large anisotropy in hydraulic conductivity [*Gelhar*, 1993; *Salehin et al.*, 2004; *Sawyer and Cardenas*, 2009; *Yager*, 1993]. *Rosenberry and Pitlick* [2009b] highlighted the importance of both vertical and horizontal flow processes in the streambed, reinforcing the need to quantify both horizontal and vertical streambed hydraulic conductivities.

Hydraulic conductivity is an essential parameter for ISSHMs, but estimating its value is probably one of the most challenging endeavors in conceptualizing streambeds in numerical models. Three main types of challenges can be identified: spatial heterogeneity, transience, and the scale dependency of any particular measurement. *Calver* [2001] reviewed dozens of measured and calibrated hydraulic conductivities of streambeds and demonstrated that values typically vary between 10^{-10} and 10^{-2} m/s. In a more recent contribution, *Stewardson et al.* [2016] compiled data from point measurements of streambed hydraulic conductivity and reported reach-average values between 10^{-5} and 10^{-3} m/s. Like *Calver* [2001], *Stewardson et al.* [2016] noted that sections of a streambed could essentially be impermeable with hydraulic conductivities as small as 10^{-10} m/s, 5 orders of magnitude smaller than the lowest reach-scale averaged value. A further challenge in assessing the hydraulic properties of streambeds is transience. Colmation processes reduce K at and near the sediment-water interface, while erosion processes tend to cause an increase of K. *Gianni et al.* [2016] compiled data of transience of hydraulic conductivity and concluded that variations up to 3 orders of magnitude can occur between erosion and deposition cycles. Finally, the approaches to estimating hydraulic conductivities operate on different spatial scales in both the vertical and horizontal directions [*Sebok et al.*, 2015]. The influence of combining measurements with different spatial scales has so far not been quantified and creates challenges for reconciliation of model with field data and vice versa.

A range of methods has been proposed to measure hydraulic conductivity at a given location directly ("point estimates"). A widely used direct method is through imposing a known hydraulic gradient between two points and then measuring the resultant fluid fluxes. The hydraulic conductivity can then be inferred through Darcy's law. This method is the underlying principle of slug tests, seepage meter tests, and permeameter tests. The advantages and disadvantages of seepage meter and permeameter tests are discussed in review papers by *Kalbus et al.* [2006] and *Landon et al.* [2001]. *Landon et al.* [2001] emphasized that if a low-permeability layer (clogging layer) is present, its position must be known for a reliable design of the test and the subsequent analysis. Practical difficulties for these methods arise in deep rivers, or in rivers with large flow velocities.

Field permeameters, seepage meters, or hydraulic gradient methods yield estimates of vertical hydraulic conductivity, while slug tests give horizontal hydraulic conductivity [*Landon et al.*, 2001]. A few methods can provide an estimate of both horizontal and vertical hydraulic conductivities. For example, *Chen* [2000] designed an L-shaped standpipe to measure horizontal hydraulic conductivity and, for the test cases presented, found that the horizontal hydraulic conductivity was 3 to 4 times larger than the vertical one. *Kelly and Murdoch* [2003] proposed the constant rate well test that allows estimation of horizontal and vertical hydraulic conductivities of sediments through inversion of an analytical solution. It is also important to note that the representative volume of these estimates is small.

The application of hydraulic approaches can also be challenging in the presence of thin clogging layers such as biofilms. An interesting approach to qualitatively identify areas of high and low hydraulic conductivities related to biological clogging was suggested by *Claret and Boulton* [2009]. They demonstrated that microbial activity and biogeochemical gradients along subsurface flow paths were smaller where hydraulic conductivity was high and vice versa. Quantifying the properties of the clogging layer is challenging, and very few studies have attempted to do so. *Blaschke et al.* [2003] and *Ulrich et al.* [2015] collected streambed samples using freezecores from a perennial river and identified clogging layers.

Freezecoring is a promising approach to obtain largely undisturbed sediment samples that can reveal the in situ heterogeneity. *Humpesch and Niederreiter* [1993] described this approach in detail and provided instructions to obtain 20 cm samples of vertical riverbed down to a depth of 10 m. In this method, liquid nitrogen is injected for 30–40 min into a hollow lance that has previously been rammed into the sediments. Alternatively, carbon dioxide can be used instead of liquid nitrogen [*Franchini and Zeyer*, 2012]. Note that freezecoring has practical limitations in rivers containing warm water as well as in compacted cobble-bed rivers. *Liernur et al.* [2017] reviewed to what extent the freezecoring process itself affected the integrity of the core and showed that there are disturbed zones in the proximity of the lance (see also Figure 2). *Strasser et al.* [2015] obtained freezecores from streambeds and built permeameters around cut-out subsections of the core, at a sufficient distance from the lance where the core was not disturbed. They measured horizontal and vertical hydraulic conductivities and compared their results with various other approaches for estimating hydraulic conductivities, including grain-size analysis (see below) as well as in situ permeameter tests. While they observed a good agreement with permeameter tests, they highlighted inconsistencies with grain-size-based approaches.

Freezecores from streambeds have also been combined with tomography techniques such as X-ray "Computer Tomography Scanning" (CT scanning) (Figure 2), which provides the information required to

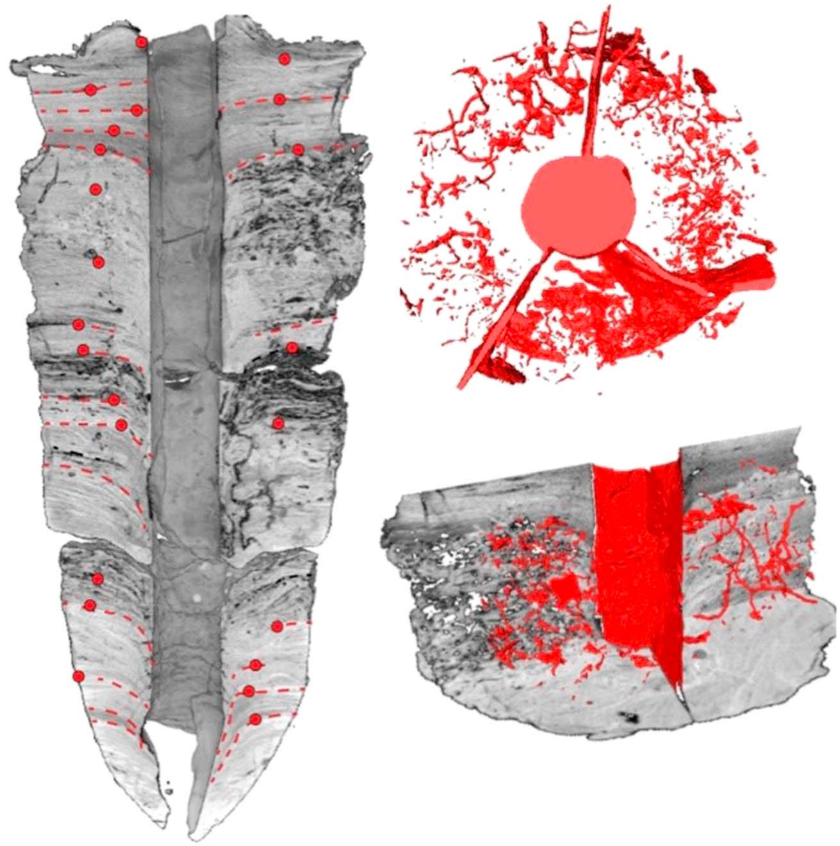

Figure 2. An example of a conductivity-temperature-depth scan of a freezecore obtained in the floodplain of a restored section of the Thur river in Switzerland. The left image shows a vertical cross-section (height: 60 cm, width: 20 cm) which allows identifying the areas that have been influenced by ramming in the lance into the streambed. The images on the right show pores with a diameter above a certain threshold of the same freezecore. The top image is a view from above; the lower image is a vertical subsection. Images on the right: *Liernur* [2016]; Image on the left: *Liernur et al.* [2017].

reconstruct "pore-scale" network models of connectivity [*Liernur*, 2016; *Liernur et al.*, 2017]. In this approach, numerous X-ray images of the sample are taken from different angles, which allows the reconstruction of a 3-D image. *Helliwell et al.* [2013] provided a review of the applications of X-ray computed tomography in soil sciences. A comprehensive overview of the principles of CT-image acquisition was provided by *Ketcham and Carlson* [2001]. In hydrology, X-ray CT-based pore networks have been used to estimate hydraulic conductivity under varying hydraulic conditions [*Périard et al.*, 2016]. Other researchers used pore-scale networks obtained from X-ray CT scans for "computational fluid dynamics" simulations. A recent special issue of the journal *Advances in Water Resources* on pore-scale modeling provided numerous examples of how such approaches can help to improve our understanding of fluid dynamics in porous media [*Lunati et al.*, 2016]. The combination of freezecoring and X-ray CT techniques paves the way for a better understanding of the pore-scale organization of sediments in the streambed. Pore-scale numerical modeling can further assist in understanding how the structure of the streambed influences the hydraulic properties on a small scale.

The grain-size distribution provides an alternative approach to estimate hydraulic conductivity, taking advantage of the intrinsic link between grain-size distributions and hydraulic properties. Relationships between hydraulic properties and grain-size distributions were recognized early in hydrological science [*Alyamani and Sen*, 1993; *Schlichter*, 1905; *Vukovic and Soro*, 1992]. However, relating hydraulic conductivity to grain-size distribution is not straightforward [*Alyamani and Sen*, 1993]. *Odong* [2007] applied different methods for the same samples and identified large variation in estimates of hydraulic conductivity. More recently, *Song et al.* [2009] determined the hydraulic conductivity in the field using permeameter tests and compared the results with estimates obtained from grain-size distributions. All grain-size-based methods overestimated the hydraulic conductivity, a result consistent with the previously mentioned study of *Strasser et al.* [2015]. A further limitation of the "classical" grain-size approaches was highlighted by *Chen* [2000], who points out that estimation of hydraulic conductivity by grain-size analysis precludes the consideration of anisotropy. Additionally, grain-size analysis cannot consider preferential pathways, which can be important in streambeds (see Figure 2 for an example).

Nevertheless, recent studies suggested obtaining grain-size distributions based on image analysis because it can provide valuable information on conductivity patterns at the top of the streambed. Image-based analysis of the top of the streambed will often have to be combined with methods that provide information on the vertical structure as well (e.g., through freezecoring) as the top layer of the streambed often features a different sedimentary composition than the underlying sediments because of armoring and other geomorphological processes. The potential for using image analysis to obtain granulometric features was discussed in *Francus* [2004]. Automated grain-size analysis approaches have since evolved rapidly, as discussed by *Cislaghi et al.* [2016]. Owing to the rapid developments of unmanned aerial vehicles (UAVs) and miniaturization of sensors and cameras, the efficiency and spatial resolution of image acquisition methods have also greatly improved, even in areas where accessibility is an issue. *Langhammer et al.* [2017], for example, repeatedly overflew river sections to identify changes in granulometry due to flood depositions. Such spatially distributed information on grain size can be integrated into geostatistical frameworks (see Tutorial 2).

Geophysical methods can also provide a map of the structure of the subsurface. Hydrogeophysical tools based on electrical resistivity and electromagnetic induction methods are gaining popularity in streambed studies [*Rubin and Hubbard*, 2005]. *Crosbie et al.* [2014] used a geophysical characterization of the streambed to evaluate information from a losing disconnected river. The spatial coverage and thickness of the riverbed clay layer, a key control on infiltration, was mapped using electrical resistivity surveys. *Wojnar et al.* [2013] undertook an assessment of geophysical surveys as a tool to estimate riverbed hydraulic conductivity. Vertical hydraulic conductivity was estimated using some methods at varied scales, including seepage meters, slug tests, and heat and water flow river-aquifer modeling. These estimates were compared with stratigraphic information using resistivity, electromagnetic, and seismic data. The paper concluded that geophysical methods could not be used alone to determine appropriate ranges of vertical hydraulic conductivity. Both hydrogeological and geophysical methods are required to determine the correlation between resistivity data and hydraulic conductivity data. *Crook et al.* [2008] installed electrodes directly into the streambed to obtain images of electrical resistivity. Their approach allowed the thickness and continuity of a highly permeable gravel layer to be mapped. *Slater et al.* [2010] combined electrical imaging with distributed temperature sensing methods to characterize river-groundwater interactions. Geophysical methods are also increasingly used to map hyporheic processes [e.g., *Ward et al.*, 2010; *Toran et al.*, 2012]. *Binley et al.* [2015] reviewed the emergence and development of hydrogeophysics, including emerging techniques and future opportunities in hydrogeophysics, for improved understanding of subsurface processes over multiple scales. Many of the ideas presented are likely to be relevant in streambed hydrological applications.

Approaches for estimating hydraulic properties based on controlled forcing to the system through abstracting groundwater, such as pumping tests, have been used for decades in hydrogeology. Such pumping tests have been further developed to provide information on the heterogeneity of the subsurface, through hydraulic tomography approaches such as those described by *Illman* [2014]. However, using pumping tests to infer streambed properties remains a challenge. An approach to rapidly identify changes in hydraulic properties across the stream-aquifer interface was proposed by *Gianni et al.* [2016]. It uses the variations of the water table measured in a piezometer close to a stream in response to changes in river dynamics. The approach is based on an analytical solution assuming a rectangular stream geometry, and that the changes in hydraulic properties are related to the deposition of fine particles or the development of biofilms, and not to significant changes in streambed topography.

Several authors have proposed a combination of methods and approaches to capture the heterogeneity of hydraulic properties and its effect on flow and transport in streambeds. *Schmidt et al.* [2006] characterized spatial heterogeneity in streambeds using measurements of streambed temperature at different depths. *Schornberg et al.* [2010] systematically evaluated the effects of streambed heterogeneity on estimates of exchange fluxes from thermal depth profiles. *D. H. Käser et al.* [2014] provided a detailed description of many aspects of streambed structure, including hydraulic conductivity, gradient, topography, and exchange fluxes. Other noteworthy examples are *Karan et al.* [2014], who measured hydraulic conductivity, temperature profiles, and hydraulic gradients at a large number of locations along the Holtum stream in Denmark. *Rosenberry and Pitlick* [2009a] measured vertical and horizontal hydraulic conductivities, seepage rates, hydraulic gradients, and shear stress and related their results to the bedforms present.

Because it exhibits such a wide range of possible physical values over short distances, measuring hydraulic conductivity remains a major challenge. The heterogeneity and anisotropy, as well as transient nature of streambeds, still cannot be captured satisfactorily with existing approaches. However, any estimate of hydraulic conductivity provides very useful information that can be integrated into geostatistical frameworks (see upcoming section on geostatistics and Tutorial 2] and provides critical information to estimate states and parameters of hydrological models. If more robust relations between grain-size analysis and hydraulic properties can be developed, image-based approaches that provide grain-size distributions across the surface of the streambed could be better integrated into such statistical analyses and the subsequent quantitative flow modeling approaches.

2.1.2. River Bathymetry

Accurate measurements of streambed bathymetry are critical for simulating a variety of hyporheic processes [*Boano et al.*, 2014]. Bathymetry is also required to simulate surface water hydrodynamics. The application of accurate bathymetric information is not limited to numerical models. For example, *Thoma et al.* [2005] compared digital elevation models created at different times for a given location and estimated sedimentary volume change over time.

Several studies demonstrated that it is possible to map streambed bathymetry through shallow water using standard photogrammetric techniques [*Carbonneau et al.*, 2006; *Westaway et al.*, 2003]. Despite promising results, *Hilldale and Raff* [2008] identified several limitations in the application of these techniques, including the different sensitivity to depth of different color bands. The limitations of other common methods (e.g., "acoustic Doppler current profiler", an acoustic method applied in *Dinehart and Burau* [2005]) are also discussed by *Hilldale and Raff* [2008] and compared to the potential of obtaining highly accurate river bathymetries over large areas using airborne lidar data (e.g., reach or even catchment scale). They demonstrated using various field cases that the quality of bathymetry was comparable to terrestrial lidar systems and river bathymetry obtained using photogrammetry.

An issue related to the successful use of lidar measurement is water clarity. According to *Hilldale and Raff* [2008], lidar can be applied to two or three times the Secchi depth. One Secchi depth corresponds to the depth where the Secchi-disk (a plain white, circular disk with 30 cm in diameter) is no longer visible to humans. In a review on mapping of river topography using remote sensing, *Feurer et al.* [2008] noted that mapping of shallow rivers also remains a challenge but points out that airborne lidar is an emerging and highly promising technique. Notably, lidar has also been used from boats [*Alho et al.*, 2009]. A key limitation of the classical lidar systems is the scatter of the signal due to the presence of water. A new generation of bathymetric lidar technology was presented by *Mandlburger et al.* [2011] to address this limitation. The laser operates in a spectral range matching the transmittance window of water and can be mounted on a small plane or helicopter. The newly developed lidar system can be applied to up to one unit of Secchi depth. The horizontal resolution is dependent on the height and speed during acquisition. Under optimal conditions, it allows the generation of streambed topography with a spatial resolution of around 20 cm by 20 cm. This resolution is, however, still insufficient for studies on invertebrates or microbial processes.

Developments in sensor technology have facilitated data acquisition for fluvial systems, as demonstrated in the review by *Marcus and Fonstad* [2008]. Sensors and data acquisition have further advanced, for example, lidar approaches [*Harpold et al.*, 2015] as well as multispectral, hyperspectral, and thermal imaging approaches [*Carbonneau and Piégay*, 2012]. Developments in UAV and sensor technologies make remote sensing approaches more cost-effective, with a higher spatial resolution, while enabling a high acquisition frequency, even at sites that are difficult to access. A high acquisition frequency is a great advantage in dynamic systems such as rivers and streams, and it enables detection of morphological changes [*Cook*, 2017]. Lidar sensors have also been miniaturized to the extent that they can be mounted on small UAV systems. For example, a UAV developed by ALTIGATOR can be equipped with a lidar developed by the company YELLOWSCAN (http://www.yellowscan.fr/news/news-release). The total weight of the entire system is only 5.6 kg, and it can fly autonomously up to 25 min. Also, high-resolution cameras can be used in photogrammetric approaches to generate digital elevation models of floodplains. An example of such data is shown in Figure 3.

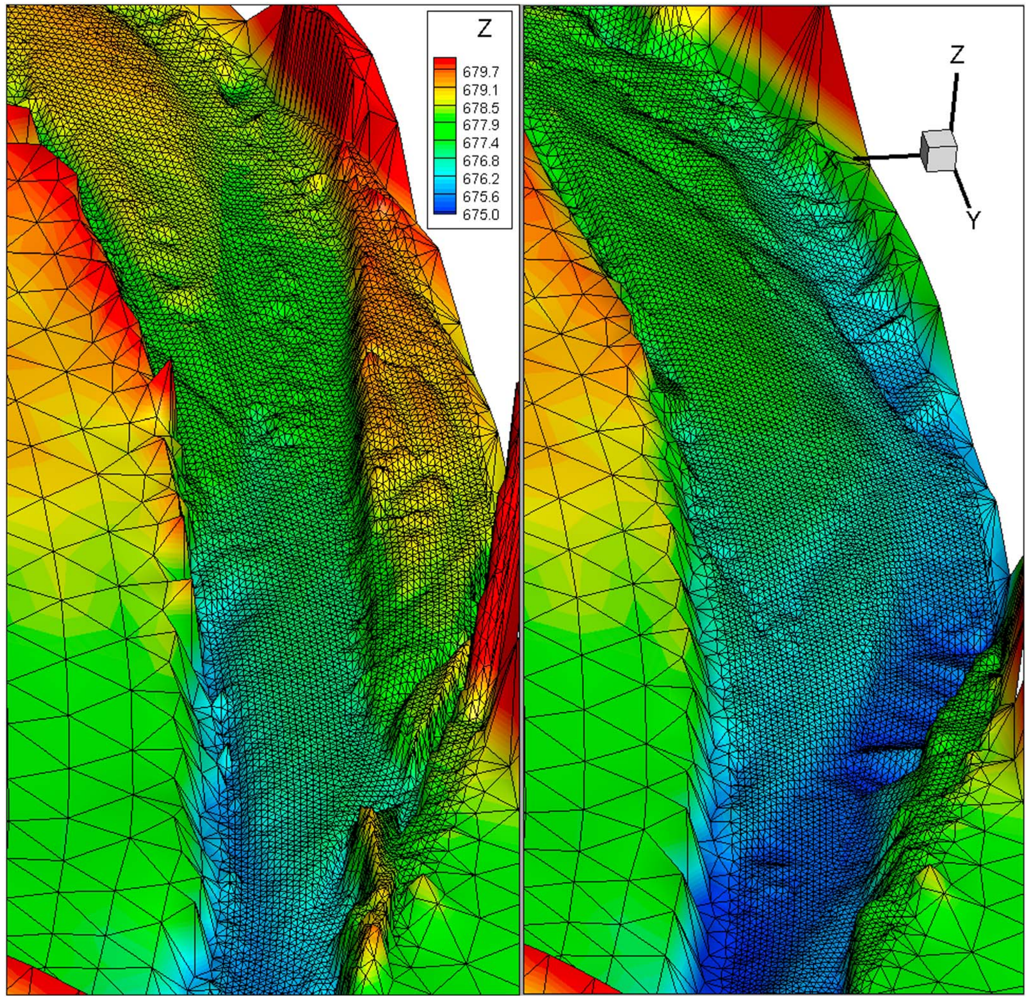

Figure 3. Topography (implemented in a numerical model) of the Emme River (meter above mean sea level), Switzerland, during low flows as an example of a UAV application. The images show a stretch 500 m long and 250 m wide. The two images are based on photogrammetry and show streambed topography (left) before and (right) after a major flood event that modified the streambed. The timing of the image acquisition was critical, as photogrammetry only works for dry streambeds and the Emme River only dries up a few days a year. UAVs provided the flexibility to acquire the data within 24 h after the river dried up. Organizing a helicopter or a plane on such short notice is often impossible.

2.2. Geostatistical Modeling of Geological Structures

Geostatistics, which is essentially advanced data interpolation, is used to represent the heterogeneity of hydraulic properties of aquifers and streambeds. New methods are being developed to model the heterogeneity of geological structures, extending the spectrum of methods that were reviewed extensively by *Koltermann and Gorelick* [1996] and *de Marsily et al.* [2005]. The development is driven by the need to produce more realistic models from a geological point of view, with a better representation of observed spatial connectivity patterns [*Gómez-Hernández and Wen*, 1998; *Zinn and Harvey*, 2003; *Kerrou et al.*, 2008; *Renard and Allard*, 2013]. Following the classification proposed by *Koltermann and Gorelick* [1996], two main types of heterogeneity models are discussed here: "structure-imitating" and "process-imitating." We focus this section on advances related to these two models that are relevant to fluvial or alluvial geological environments and that have been published after 2005.

2.2.1. Structure-Imitating Models

"Structure-imitating models" are based on stochastic and geometric techniques and aim to reproduce structures and patterns observed in the field. An example in this category are "object-based models." While the first object-based models used simple objects such as ellipses to represent geological structures [*Allen*, 1978; *Jussel et al.*, 1994], recent models include much more complex parametric shapes and

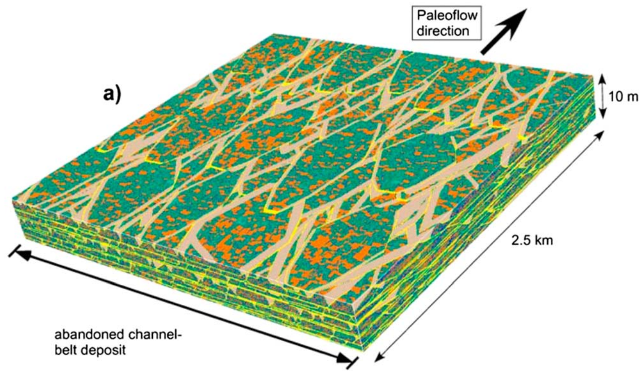

Figure 4. An example of simulated heterogeneity for a braided river system modeled by the method of *Ramanathan et al.* [2010]. Image from *Ramanathan et al.* [2010]. The yellow color represents boundaries of units of the highest hierarchical levels. The unit bars are represented in orange color. The other colors are used to visualize the different sedimentological units.

relationships between objects. In one example, *Ramanathan et al.* [2010] modeled braided rivers by stacking archetypal polyhedrons for the different sedimentological units in the system and used a hierarchy of scales (Figure 4). The relationship between the various scales and units is chosen to mimic field observations. The method allows the integration of a broad spectrum of knowledge for a given type of sedimentological environment. However, it requires specific developments for each type of sedimentological environment and cannot easily be conditioned to borehole or geophysical data. As a result, practitioners generally use other methods.

One of the most widely used alternatives to object-based models in hydrogeology is T-PROGS, which stands for Transition PRObability Geostatistical Software [*Carle and Fogg*, 1997]. T-PROGS is designed for the geostatistical analysis and stochastic generation of geological units, also called facies. T-PROGS first calculates the transiograms, which is the probability of transition between facies, using borehole data or outcrop observations. In the context of river-groundwater interactions, geophysical surveys and freezecores (see section 2.1) can also provide facies information to generate transiograms. With the transiograms, multidimensional sequences of geological facies can then be simulated. T-PROGS has been the most extensively used method in the context of large-scale (e.g., catchment scale) river-groundwater interactions over the last years [*Engdahl et al.*, 2010; *Fleckenstein et al.*, 2006; *Frei et al.*, 2009]. It is flexible, rather simple to implement, and can be easily conditioned to field observations [*Fogg et al.*, 2000; *Fleckenstein and Fogg*, 2008; *Weissmann et al.*, 2015].

T-PROGS can generate artifacts when simulating facies because it uses indicator cokriging. The multinomial categorical simulation has been developed to avoid these artifacts [*Allard et al.*, 2011], but it has not yet been applied to river-groundwater interaction studies. Another alternative to T-PROGS is the "Plurigaussian model" [*Armstrong et al.*, 2003], which offers greater control on the relationships between the geological facies as well as on trends of proportions of facies. The Plurigaussian model is an extension of the "truncated Gaussian technique" [*Matheron et al.*, 1987] that has been used recently to generate heterogeneity patterns and investigate their impact on hyporheic flow using both numerical and laboratory experiments [*Fox et al.*, 2016]. *Mariethoz et al.* [2009] presented an application of the plurigaussian model to a fluvial environment.

Among the "structure-imitating models," "Multiple Point Statistics" (MPS) offers an interesting alternative [*Comunian et al.*, 2012; *Hu and Chugunova*, 2008; *Straubhaar et al.*, 2011; *Strebelle*, 2002; *Mariethoz and Caers*, 2015]. It is more flexible than the object-based models and allows the generation of conditional simulations that can reproduce a wide range of realistic geological structures. In practice, the user must provide a training image, which corresponds to a conceptual geological model. In 2-D, the training image represents the spatial patterns that are expected to occur. It can be drawn by hand, derived from field observations at an analog site (e.g., Figure 5), or obtained by another model. For example, the 3-D block obtained by the technique of *Ramanathan et al.* [2010] and displayed in Figure 4 could be used as a training image. Also, image analysis combined with grain-size analysis (see section 2.1) could form the basis to generate a training image for spatial patterns of riverbed hydraulic conductivity. The training image is much richer than any covariance or two-point based transition probabilities model. MPS consists of deriving high-order statistics from the training image and then simulating random fields. These fields can be conditioned to local or global data such as probability maps derived from geophysical surveys [*Straubhaar et al.*, 2016] or hydraulic conductivity measurements at different scales, which for riverbeds could range from freezecores to pumping tests. Figure 6a shows one realization obtained using the Direct Sampling MPS method [*Mariethoz*, 2009] with the training image displayed in Figure 5. Figure 6a illustrates that the channels of high conductivity (shown in white) are well connected. Traditional geostatistical techniques allow to accurately reproduce the

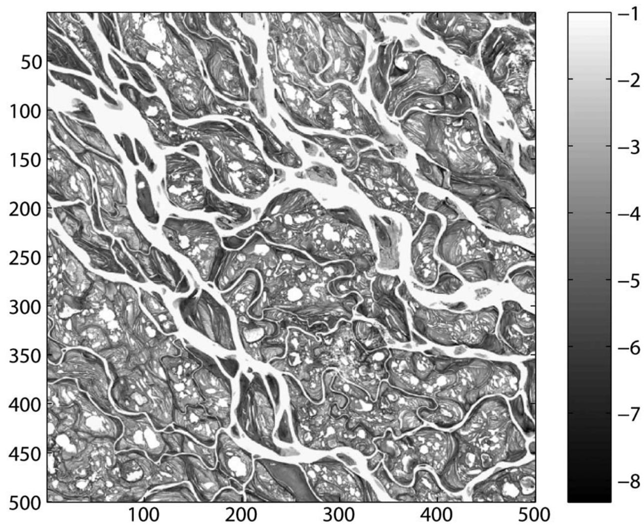

Figure 5. Training image derived from a Landsat 7 image of the Lena Delta (Russia). The coordinates are expressed in number of pixels. The gray scale represents the $\log_{10}$ of hydraulic conductivity values derived from the satellite image. This is a conceptual model of possible geological heterogeneity used to demonstrate the application of Multiple Point Statistics (see Figure 6). Image from *Mariethoz* [2009].

histogram and variogram of the original image but without generating the high connectivity (see Figure 6b). The two simulations have the same first-order statistics (Figures 6c and 6d), but if used as input for flow and transport simulations, they behave very differently (Figures 6e, 6f, and 6g) as shown by *Mariethoz* [2009]. Furthermore, obtaining or designing the training image for a specific case can be a practical limitation.

One of the main interests in the MPS approach is that it can be used to generate a heterogeneity model directly based on detailed mapping of sedimentary structures. For example, *Bayer et al.* [2011] mapped the heterogeneous distribution of fluvioglacial deposits in a gravel pit close to Basel, Switzerland, at the scale of several meters with a resolution of 5 cm. Based on these data, *Comunian et al.* [2011] generated realistic 3-D models of heterogeneity using a combination of classical geostatistics and MPS. Similarly, new ways of acquiring data from digital outcrop mapping with lidar can be integrated into that approach [*Klise et al.*, 2009; *Pickel et al.*, 2015].

2.2.2. Process-Imitating Models

"Process-imitating models" offer another alternative to simulate the heterogeneity of aquifers or streambeds [*Coulthard and Van de Wiel*, 2012]. A rather diverse set of process-imitating models has been developed. Some are focused on the evolution of the geomorphology of the system [e.g., *Davy and Lague*, 2009] and model the processes of erosion/transportation at the scale of the landscape. Other models have been developed to describe the final heterogeneity of the aquifer. Solving the complete set of flow and erosion-deposition equations at the catchment scale with the appropriate paleo-boundary conditions is extremely demanding, and approximate solutions have been proposed. For example, *Anderson et al.* [1999] used a random walk algorithm to generate two-dimensional braided river channel patterns through time. *Teles et al.* [2001] have developed an "agent-based model" for the simulation of fluvial systems and applied it to the Rhône River in France.

More recently, event-based models were proposed for meandering systems. They mix "process-based" equations describing the movement of rivers with simple probabilistic rules and sedimentary concepts [*Cojan et al.*, 2004; *Lopez et al.*, 2001; *Pyrcz et al.*, 2009]. The geometry of the resulting three-dimensional models (Figure 7) is controlled by parameters such as the rate of aggradation, the sediment load, or the slope of the alluvial plain.

MPS can also be used within a process-imitating model to extract spatiotemporal statistics from a series of successive lidar measurements of the topography of an active braided system. This can be used then to simulate the evolution of realistic successive topographies [*Pirot et al.*, 2014]. The technique can be combined with principles of sediment transport, erosion, and deposition to mimic the formation of a braided deposit and the resulting heterogeneity [*Pirot et al.*, 2015a].

2.3. Field Approaches for Assessing Hydrodynamics and Exchange Fluxes

2.3.1. Measuring Stream Stage, Depth, and Volumetric Discharge

Parameters such as stream stage (the elevation of the water table in the stream at a given location), depth, and discharge are essential for capturing stream dynamics. Stream depth can be calculated from the stream stage if the bathymetry of the stream is known. From a modeling point of view, stream stage is the surface domain analog to hydraulic head in the subsurface. The discharge of a stream provides crucial information

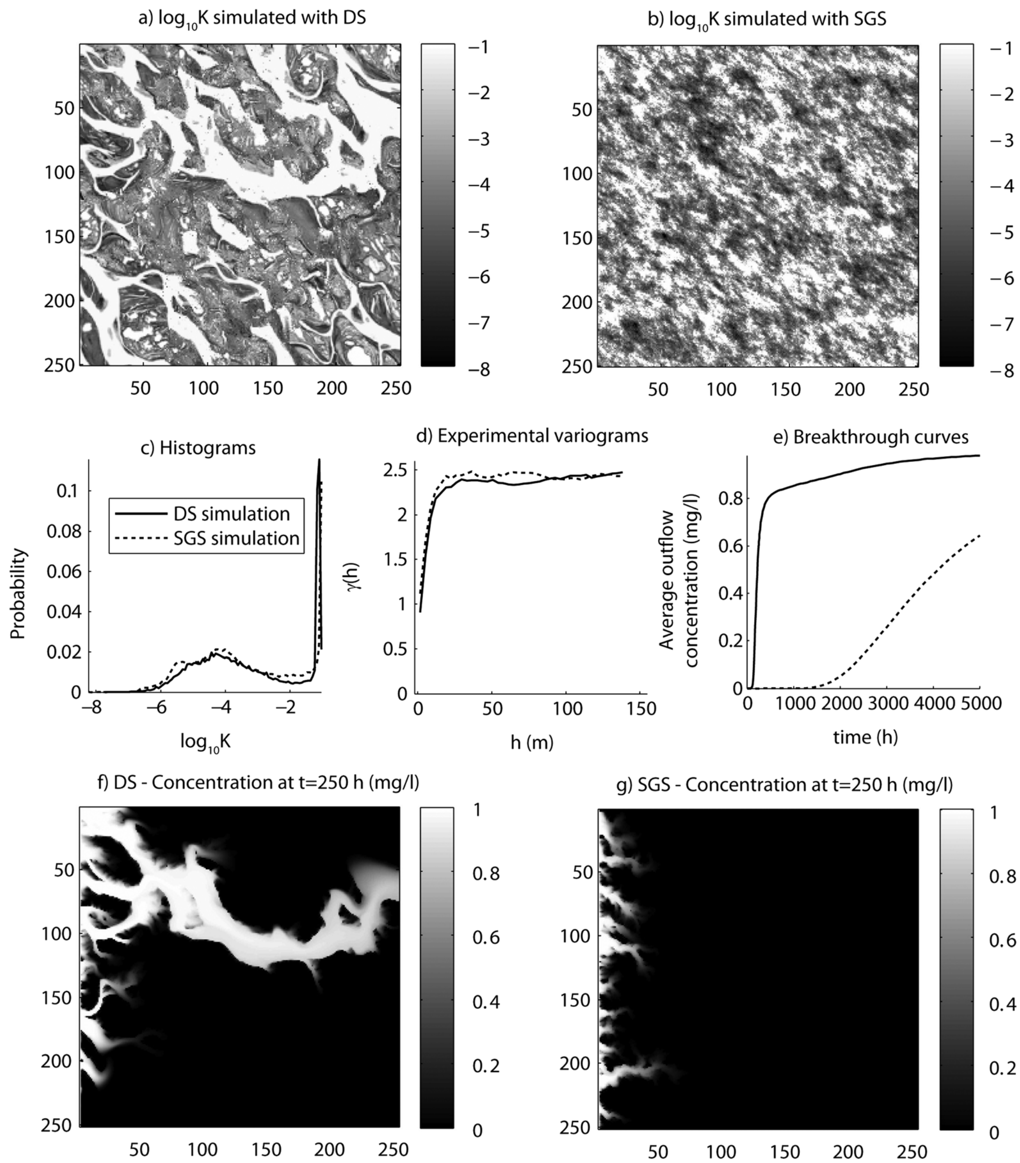

Figure 6. Comparison between Multiple Point Statistics and variogram based geostatistics. (a) One simulation obtained with the Direct Sampling (DS) MPS method. The gray level represents the value of the $\log_{10}$ of the hydraulic conductivity in m/s. (b) One simulation generated using Sequential Gaussian Simulation (SGS). (c) Comparison of histograms of simulated values. (d) Comparison of experimental omnidirectional variograms. (e) Comparison of contaminant break-through curves at the outflow boundary. The contaminant is flowing from the left to the right. (f and g) Comparison of the maps of contaminant distribution at $t = 250$ h, for the case that contaminants were injected along the left boundary (inflow boundary) at $t = 0$ h. The gray color legend represents the contaminant concentrations. Images and caption text slightly modified after *Mariethoz* [2009].

on the water balance of a catchment. Furthermore, discharge is of critical importance for sediment and erosion processes.

Measuring stream depth in the field is straightforward, with electronic pressure transducers and loggers, and new and inexpensive designs are continuously being developed [e.g., *Greswell et al.*, 2009; *Riley et al.*, 2006]. The project "crowdwater" (crowdwater.ch) hosted by the University of Zurich provides a Web-based service to allow anyone to collect, via a smartphone app, hydrological data such as water levels, streamflow, and soil moisture.

Marcus and Fonstad [2008] reviewed key papers dedicated to the application of remote sensing for measuring stream depth. Estimating depth using remote sensing creates several challenges, and it appears that its

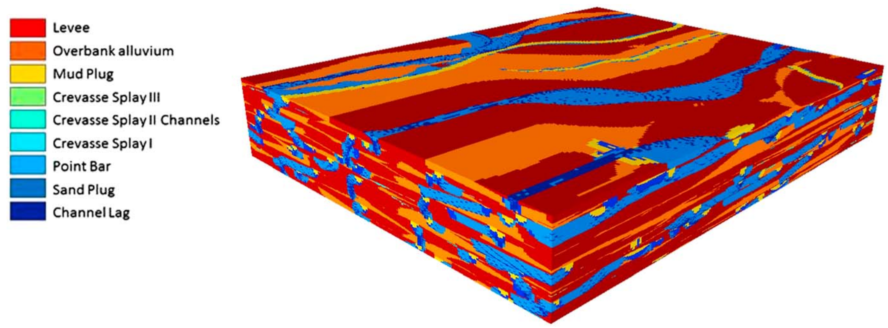

Figure 7. An example of a 3-D simulation of a meandering system using the events-based model of *Lopez et al.* [2001]. Image source modified after *Linde et al.* [2015].

application has been, until now, not straightforward. Irregular channel morphology, substrate, and in-stream vegetation are some of the factors that complicate the analysis. *Yan et al.* [2015] compiled current and past satellite missions that can be used for flood extent monitoring and stream stage, with a focus on coarse resolution (>10 m) and low-cost remote sensing data. *Jiang et al.* [2017] provided a comprehensive review on satellite-based radar altimetry, with a focus on the hydrological applications of CryoSat2. This satellite is very interesting because it operates with a narrow intertrack distance of 7.5 km at the equator, allowing for a much higher spatial resolution compared to other satellite-based altimetry approaches. On the downside, the repeat orbit of this satellite is 369 days, which is significantly longer than the short repeat orbits of other satellites [*Jiang et al.*, 2017]. A comprehensive review of satellite altimetry missions with a compilation of precisions and biases is provided by *Asadzadeh Jarihani et al*. [2013]. *Grimaldi et al.* [2016] also reviewed medium- to high-resolution (centimeter-resolution) remote sensing-based approaches (including spaceborne and airborne) on water levels in the context of flood modeling. Both satellite and airborne altimetry can be integrated into data-assimilation approaches (see section 3.1).

A range of classical approaches are available to estimate discharge, including dilution gauging, velocity-area methods, or direct volumetric measurement for small streams [*Dingman*, 2014]. *Rantz* [1982] provided a comprehensive overview and discussion of numerous methods that allow discharge to be quantified. If rating curves (e.g., the relation between stream depth and discharge) are available, discharge can be calculated using stream stage.

Lidar has been successfully used to model rating curves of streams. *Nathanson et al.* [2012], for example, estimated rating curves with a fluid mechanics-based model constrained with topographic data from an airborne lidar scanning. Similarly, *Lyon et al.* [2015] investigated the potential for airborne laser scanning to derive stream rating curves. They concluded that it is theoretically possible to derive rating curves based on lidar data. Lidar systems are now available that can be mounted to UAVs, therefore greatly increasing the applicability of lidar approaches (see section 2.1).

An innovative approach to measure discharge based on surface flow velocity was developed by the PHOTRACK company (http://www.photrack.ch/what.html). Their approach uses webcams and smartphones that extract surface flow velocities using 3-D particle tracking approaches. By integrating ordinary mobile phones, available data on discharge measurements can be significantly increased, especially through citizen science, the collection, and analysis of scientific data by members of the community, often working on a project in collaboration with scientists (see, for example, the project video for the Themi River Catchment in Tanzania https://www.youtube.com/watch?v=WUDIVXvGeOI).

2.3.2. Estimation of Exchange Fluxes Between Rivers and Groundwater

Estimating exchange fluxes—the exchange of water (e.g., volumetric flow rate or flux) between groundwater and a river (and vice versa)—is important for many reasons. Groundwater fluxes into surface water systems are important for supporting ecological habitats in rivers [*Boano et al.*, 2014]. Groundwater fluxes also influence the flow regime, which is a master driver of processes and biota in rivers, riparian zones, and floodplains [*Poff et al.*, 2010]. In summer, base flow derived from groundwater can often be the most significant component of river flow [*Cook*, 2013]. Losing rivers can provide an important focused point source of recharge to the groundwater system [*Winter et al.*, 1998].

From a modeling perspective, information on the rate of volumetric water exchange can be used to calibrate and constrain hydrological models. Flux can be computed using Darcy's law, through knowledge of hydraulic conductivity and head gradient. Measuring this exchange flux independently or directly offers the advantage that hydraulic conductivity does not need to be known a priori. Similarly, determining a flux independently or directly contributes to constraining a model. Exchange fluxes can be simulated directly in a model (e.g., simulating solute transport in the model directly) or indirectly (by computing the flux outside the model using independent methods and then comparing the results with the modeled fluid flux). Tutorial 3 provides an example. Finally, a knowledge of exchange flux between groundwater and a river offers the potential advantage that it will average over larger scales as the measurement usually is representative of larger scales, such as the reach scale or catchment scale (see Figure 1).

There is a variety of methods available for estimating exchange fluxes between a river and aquifer [*Cook*, 2013; *Rosenberry and LaBaugh*, 2008]. Each method will have an inherent level of uncertainty, and the critical issue is to determine an appropriate level of uncertainty in a specific application. The most reliable and robust approach likely depends on the spatial scale of the application as well as the specific research question. Framing each problem and investigation in the context of a clear scale requirement is prudent. Available methods to estimate exchange fluxes include seepage meters, monitoring wells, and thermal methods [*Rosenberry and LaBaugh*, 2008]. These methods typically apply at small scales on the order of meters. The approaches outlined in this section cover all scales: at the very local scale flux estimates can be made using a seepage meter; at the river/reach scale using tracers and stream gauges and at the regional scale using river-groundwater interaction models. Similarly, we can also distinguish hydraulic and tracer/chemical-based approaches.

Seepage meters represent a hydraulic approach to measuring "point-scale" river-groundwater exchange flux. *Rosenberry and LaBaugh* [2008], similar to *Murdoch and Kelly* [2003] and *Shinn et al.* [2002], point out that hyporheic exchange fluxes complicate the interpretation of flux measurements with seepage meters in flowing water. The reason is that water discharging into the river can be either groundwater, re-emerging river water, or a mixture of both [*Kalbus et al.*, 2006]. New designs are being developed to reduce the effect of reemerging water [e.g., *Rosenberry*, 2008]. Studies using seepage meters also reveal very large variations in the values of fluxes that may be measured in both spatial (over meters) and temporal (over days and weeks) terms in a given river or wetland system. Reconciling local measurements with the larger-scale (e.g., catchment-scale) water balance remains a challenge.

Batlle-Aguilar and Cook [2012] studied a larger reach scale using a hydraulic approach, which consisted of blocking off a section of a stream and adding water to the stream to induce a head gradient and measure infiltration loss. It is expected that their measurements are far more reliable and representative of the infiltration across a larger area than measurements made at a very local scale using an infiltrometer or seepage meter. The approach has some practical limitations, such as the need for a large volume of water, as well as the impact of blocking off a stream for any downstream user. There are also expected to be logistical challenges and limitations applying this method on large/wide rivers where there is a significant pre-existing flow rate.

Tracer/chemical-based approaches provide an alternative to hydraulic-based approaches for flux estimations. *Cook* [2013] reviewed methods for estimating groundwater inflow to rivers using river chemistry surveys. He concluded that environmental tracer methods can provide sound estimates of groundwater discharge at a scale and accuracy that is not possible with most other methods. The tracers that have been employed include electrical conductivity (EC), stable isotopes of deuterium and 18-O, chlorofluorocarbons (CFCs), and 222-Radon. The successful application of the tracer approach for estimating exchange fluxes requires a significant difference in tracer concentration between groundwater and river water. Depending on the tracer used, it is theoretically possible to resolve groundwater discharge rates as low as 2–5 mm/d using a chemical tracer approach [*Cook*, 2013].

Automated and semiautomated continuous sampling allows river chemistry and hydraulics to be measured at unprecedented spatial and temporal scales. It is now relatively straightforward for continuous sampling systems to provide information on river stage, EC, pH, temperature, and dissolved oxygen. Studies now use transient information for tracers such as EC [*Vogt et al.*, 2010] and radon [*Stieglitz et al.*, 2010] to quantify the nature of river-groundwater interaction and associated exchange fluxes. A continuous automated

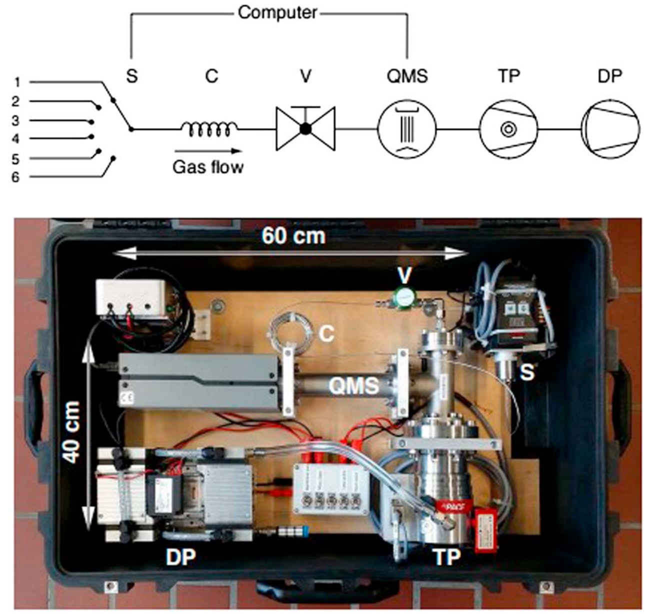

Figure 8. Figure and figure caption obtained directly from *Brennwald et al.* [2016]. (top) Schematic overview and (bottom) photo of the miniRuedi mass-spectrometer system (see also Table 1): 6-port inlet selector valve (S), capillary (C), inlet valve (V), quadrupole mass spectrometer (QMS), turbomolecular pump (TP), and diaphragm pump (DP). The inlet selector valve and the quadrupole mass spectrometer are controlled by a computer. The photo shows the miniRuedi mounted in a wheeled hardshell suitcase for transport and protection.

sampling of other tracers such as CFCs and 14-C is currently not possible but is a key area for future development. The use of multiple tracers, sampled continuously through time, will provide important information with which to constrain and test models of river-groundwater interaction.

Brennwald et al. [2016] developed a new system for on-site environmental gas analysis (Figure 8). They developed a portable (i.e., it can be easily carried by two people) and autonomous mass spectrometric system ("miniRuedi") for quantification of the partial pressures of He, Ne (in dry gas), Ar, Kr, N_2, O_2, CO_2, and CH_4 in gaseous and aqueous matrices in environmental systems. The utility of this system was illustrated in applications relating to lake-atmosphere exchange and gas emissions from the seafloor. With an analytical uncertainty of 1–3%, this portable and autonomous device opens up enormous possibilities for measuring gas tracers in riverbed systems as a necessary precursor for estimating properties of the riverbed itself and river-groundwater exchange.

Heilweil et al. [2016] examined methane emissions in a coastal plain stream. They injected dissolved gasses (methane and krypton) into the stream to quantify methane losses at the catchment scale, thereby illustrating the utility of dissolved-gas tracers for estimating stream methane fluxes at a larger catchment-scale in contrast to point-scale measurements.

Interpretation of temperature data is becoming commonplace in quantitative river-groundwater interaction [e.g., *Vogt et al.*, 2012; *Hatch et al.*, 2006; *Keery et al.*, 2007; *Molina-Giraldo et al.*, 2011], and new technologies are therefore applied to measure stream temperature. For example, "Fiber-optic Distributed Temperature Sensing" allows temperature to be measured along an optical fiber of up to several kilometers in length (and therefore up to the reach scale) with a spatial resolution of about 1 m and a temporal resolution on the order of minutes. Examples of this technology applied to river-groundwater interactions were given in *Henderson et al.* [2009], *Selker et al.* [2006], and *Tyler et al.* [2009].

Besides being a key factor for stream ecology [*Caissie*, 2006], the thermal regime of a river can also be used to quantify the interaction between the river and the aquifer. The potential and limitations of such thermal methods were discussed in a series of review articles [*Anderson*, 2005; *Constantz*, 2008; *Stonestrom and Constantz*, 2003; *Webb et al.*, 2008], and a special issue of *Hydrological Processes* was dedicated to thermal methods in river-groundwater interaction [*Hannah et al.*, 2008]. As pointed out by *Cardenas et al.* [2008], most previous studies considered a few point measurements of temperature and assumed that these values are representative for the entire stream. The scale issue is key again. Recent technological advances allow this assumption to be overcome and to work at the necessarily larger scales. Airborne thermal remote sensing has successfully been applied in some studies [*Cherkauer et al.*, 2005; *Loheide and Gorelick*, 2006; *Torgersen et al.*, 2001]. Airborne data allow mapping the spatial distribution of temperature along the stream. *Webb et al.* [2008] cited studies that address issues associated with image calibration and spatial resolution in the context of airborne thermal mapping. An additional limitation of airborne methods is that data represent the top of the water column. If the stream is not well mixed in the vertical direction, the measurements must be interpreted with care. This issue is expected to be especially severe in large rivers that stratify. Measurements of temperature profiles in the river can provide some indication on the vertical mixing of rivers. *Munz et al.* [2016] determined the geometry of subsurface water flow around in-stream geomorphological structures by analysis of riverbed temperatures. They concluded that by using measured temperature time series in vertical profiles, the method has strong potential for characterizing the spatial patterns and temporal dynamics of complex subsurface flow geometries.

Schneidewind et al. [2016] developed a new one-dimensional approach to quantify vertical water flow in streambeds using temperature data from different depths. Using additional analyses, nonvertical components of flow could be quantified.

Recently, *Xie et al.* [2016] examined the uncertainty of different tracer methods in a large river system for estimating river-groundwater interaction. Results showed that temperature and radon profile methods are complementary at a given point, but that river chemistry methods are superior to temperature methods at the reach scale.

More generally, it is worth noting that several authors have studied river-groundwater interactions using combinations of approaches. *González-Pinzón et al.* [2015] compared multiple approaches to quantify GW-SW exchange at multiple scales. *Rosenberry et al.* [2016] combined temperature-based methods with seepage-meter measurements to constrain streambed thermal parameters and refine temperature-based values.

At the reach scale, river gauging stations may provide an appropriate approach to determine the fluxes that exist along the river reach. Tracer and velocity gauging methods are briefly reviewed in *Kalbus et al.* [2006]. Recent examples and discussions of the challenges of inferring river-groundwater interaction through discharge measurements can be found in *Payn et al.* [2009] and *Ruehl et al.* [2006]. A noteworthy development in many countries is that data of thousands of stream gauges are available, many of them in real time. For example, in the U.S., such data are available at the following link: https://waterdata.usgs.gov/nwis/sw. An informative document providing an overview of applications using such data is found at https://pubs.usgs.gov/fs/2012/3054/fs2012-3054.pdf. For Switzerland, a website of the environmental office provides real-time data of several hundred discharge stations, as well as historical data and a comprehensive statistical analysis including return periods (http://www.hydrodaten.admin.ch/de/stationen-und-daten.html). Many other countries provide similar services, including New Zealand, Australia, Canada, and numerous European countries. Such real-time data provide useful information on catchment dynamics and can be combined with data assimilation methods (see section 3.1).

3. Current Conceptualization of Streambeds in Integrated Surface and Subsurface Hydrological Flow Models

The integrated surface and subsurface hydrological flow models mentioned in the introduction, which are based on the *Freeze and Harlan* [1969] blueprint, have the capability to account for heterogeneous surface and subsurface properties. Tutorial 1 illustrates the example of the numerical model HydroGeoSphere [*Therrien et al.*, 2009; *Aquanty*, 2016] and shows how such models are conceptualized. However, the spatial discretization for large-scale (e.g., catchment scale) simulations is often too coarse to represent streambed heterogeneity [*D. Käser et al.*, 2014]. Streambeds are thus implicitly assumed to be homogeneous. Even in small-scale simulations (e.g., reach scale or hyporheic scale), streambed heterogeneity is mostly ignored except for a small number of notable exceptions such as the work presented by *Cardenas et al.* [2004], *Fleckenstein et al.* [2006], *Frei et al.* [2009], *Irvine et al.* [2012], and *Bardini et al.* [2013].

In addition to studies that focused on fluid flow, other model applications investigated the impact of streambed heterogeneities on mass or energy transport. *Brookfield et al.* [2009] applied an integrated surface and subsurface hydrological flow model, HydroGeoSphere, to simulate fluid flow and heat transport in a river reach. They represent the streambed material with homogeneous hydraulic properties. They compared simulated to observed riverbed temperatures and concluded that the calibration of their model could be improved by incorporating small-scale heterogeneities. *Schornberg et al.* [2010] simulated the influence of streambed heterogeneity on heat transport and demonstrated that although mild heterogeneity can be represented with a uniform model, pronounced heterogeneity of streambeds must be accounted for in a model to characterize water exchange between surface and subsurface properly. *Kurtz et al.* [2014] presented riverbed heterogeneity for the simulation of flow and heat transport between the river Limmat (Switzerland) and the aquifer. The interaction was calculated by a one-way coupled model and heterogeneity was represented by a limited number of zones (five) which had different riverbed hydraulic conductivities. In this specific case, temperature data contributed less to improving characterization of riverbed hydraulic conductivities than groundwater levels.

3.1. Calibration and Uncertainty Characterization of ISSHM

As it is not possible to characterize environmental systems perfectly, ISSHMs require calibration [*Anderson et al.*, 2015]. The prediction of groundwater flow with a numerical simulation model therefore requires first to solve an inverse problem where the available observations are used to estimate unknown parameters such as hydraulic conductivity or surface roughness of the streambed.

Carrera and Neuman [1986] formulated a statistical framework for calibrating different types of parameters which can be applied to the calibration of large-scale groundwater and river flow models (e.g., catchment scale) where the number of parameters to be estimated is less than the number of data points. When there are more parameters than data points, the inverse estimation problem is not well posed and unstable unless some mathematical regularization method is employed. In the 1980s, the geostatistical approach was developed and provided an alternative approach for model calibration. Posing inverse problems in a geostatistical framework can avoid problems with unstable and nonunique solutions [*Kitanidis and Vomvoris*, 1983]. Further building on the geostatistical approach, Monte Carlo (MC)-type inverse modeling methods were developed. These methods generate multiple equally likely solutions to the inverse problem, conditioned on state and parameter measurements. Examples are the sequential self-calibration method [*Gomez-Hernandez et al.*, 1997] and the Pilot Points Method [e.g., *Lavenue et al.*, 1995]. However, although MC-type inverse methods are suited for calibration of river-groundwater models, none of these methods has been extended to handle coupled river-groundwater models. The reason being that adjoint state equations from the ISSHM have to be derived and solved to calculate the derivatives of the objective function with respect to the parameters in an efficient way. Deriving and solving adjoint state equations is a formidable task for ISSHM. Therefore, alternative calibration methods, which do not require derivatives of an objective function with respect to parameters, are of interest.

Data assimilation (DA) methods assimilate measurement data sequentially (instead of simulating them in a batch, like inverse modeling methods) and are less affected by overparameterization. These methods can also be used for parameter estimation. The most prominent DA method, the ensemble Kalman filter (EnKF) [*Evensen*, 1994; *Burgers et al.*, 1998], relates measurement data (like hydraulic head, groundwater temperature, river discharge, and/or soil water content) to model states (e.g., matric potential and river levels) and model parameters (e.g., hydraulic conductivity and leakage coefficients) with help of a covariance matrix, which is estimated numerically from a large number of stochastic realizations. If measurement data do not contain information on certain states or parameters, for example, because those states and parameters are far separated in space from the measurement locations, covariances are close to zero, and those measurement data will not update the states and parameter values. The advantage of EnKF and other DA techniques is that the full posterior probability density function of all states and parameters is determined, at a relatively limited cost compared with inverse MC techniques [*Hendricks Franssen and Kinzelbach*, 2009].

EnKF (and other DA techniques) have two further advantages over inverse modeling methods. First, measurements that become available in real time can be assimilated in an online river-groundwater model. Models calibrated with historical information tend to deviate from the measured values when applied to true prediction exercises. Second, DA techniques also allow updating parameters that vary over time. A prominent example for river-groundwater models is the leakage coefficient, which is subjected to temporal variations related to, for example, floods. *Kurtz et al.* [2012] investigated to what extent EnKF can update time-dependent leakage coefficients. They used EnKF in combination with adaptive inflation [*Anderson*, 2007] and found that EnKF, with some delay, can detect temporal changes of riverbed hydraulic conductivities. However, very fast and short-term changes would remain undetected. Although EnKF is robust against nonlinear model dynamics and non-Gaussianity of the states and/or parameters (because the linearization is made over the ensemble and not around the optimum, see *Nowak* [2009]), its performance is only optimal for linear Gaussian models.

Different methods have been reported in the literature that would be able to calibrate also non-multi-Gaussian distributions of riverbed properties, as can be generated by MPS. Examples are the conditional probabilities method [*Capilla et al.*, 1999], the gradual deformation method [*Hu*, 2000; *Hu et al.*, 2001; *Jenni et al.*, 2007; *Capilla and Llopis-Albert*, 2009], the probability perturbation method [*Caers*, 2003; *Caers and Hoffman*, 2006], and the representer method extended to handle multimodal transmissivity distributions [*Janssen et al.*, 2006]. *Janssen et al.* [2006] estimated jointly hydraulic conductivities and the leakage between aquifers, which is an estimation problem not very different from a river-groundwater problem. More recent developments include the moving window approach [*Alcolea and Renard*, 2010], the iterative spatial resampling [*Mariethoz et al.*, 2010], and the ensemble pattern matching method [*Zhou et al.*, 2012; *Li et al.*, 2015]. A detailed bibliographical review about those methods is given by *Linde et al.* [2015]. Concerning sequential data assimilation methods, some promising results have been achieved with EnKF for non-multi-Gaussian parameter fields for groundwater flow [*Sun et al.*, 2009; *Zhou et al.*, 2011; *Li et al.*, 2012; *Xu et al.*, 2013], with better results as compared to classical EnKF. The particle filter [*Gordon et al.*, 1993] is an interesting alternative that allows the optimal combination of river-groundwater model predictions and measurement data, for arbitrary parameter distributions and strongly nonlinear models.

Some studies estimated the properties of spatially heterogeneous riverbeds with EnKF. All these studies focused on the reach scale (approximately kilometer scale in these cases). *Hendricks Franssen et al.* [2011] assimilated groundwater level data with the help of EnKF and updated both hydraulic conductivities and leakage coefficients for five different zones for the upper Limmat valley aquifer in Switzerland. Leakage coefficients were also estimated by EnKF for a limited number of zones by *Rasmussen et al.* [2015, 2016]. They also showed in a synthetic setup an improved characterization of leakage coefficients with this method. Other studies estimated spatial distributions of leakage coefficients. *Kurtz et al.* [2013] showed that spatially variable distributions of leakage coefficients can be updated with EnKF by assimilating groundwater level data and that the characterization of river-aquifer exchange fluxes is more improved with this simulation strategy than updating leakage coefficients for a few zones in which the river reach is divided. Finally, *Tang et al.* [2015] also estimated spatially variable distributions of leakage coefficients by assimilating groundwater level data with EnKF in a synthetic study. In this case, it was investigated whether non-multi-Gaussian patterns of leakage coefficients could be identified with groundwater level data and whether the spatial pattern of the leakage coefficients was important for the stream-aquifer exchange. *Tang et al.* [2015] found that the spatial orientation of the leakage coefficients had a relatively minor influence on the river-aquifer exchange fluxes and that an erroneous assumption of a multi-Gaussian distribution (instead of the true non-multi-Gaussian distribution) of leakage coefficients had only a slightly negative impact on the system analyzed.

Other data assimilation studies for integrated surface-subsurface flow models did not estimate leakage coefficients but showed the potential of other data for improving the modeling of surface-subsurface flow. In particular, the assimilation of river discharge was used to update the states of both the surface and subsurface domain. Given the fact that only states are updated and not parameters in these applications, the main potential lies in the short-term improvement of predictions. EnKF was, for example, applied in combination with the integrated hydrological model CATHY (CATchment Hydrology). This model simulates two-way interactions between groundwater flow and surface water flow [*Paniconi and Wood*, 1993]. *Camporese et al.* [2009] assimilated streamflow data and pressure head data in a synthetic experiment (small catchment scale of ~1 km) and found that although discharge data are important for improving river states, the characterization of pressure distributions in the subsurface was hardly improved by it. *Pasetto et al.* [2012] reached a similar conclusion for a similar synthetic v-titled catchment example; in this case, sequential data assimilation was performed by the particle filter. *Bailey and Bau* [2010] followed a different approach and also updated hydraulic conductivities. They used the Ensemble Smoother to assimilate measurements. The Ensemble Smoother can be seen as an extension of EnKF because measurements from multiple time steps (including past time steps) are used simultaneously for conditioning. *Bailey and Bau* [2010] did not use a fully coupled model and assimilated piezometric heads, cumulated groundwater return flows, and hydraulic conductivity data. This study was for a river reach of ~1 km length. In a follow-up work, *Bailey and Bau* [2012] used the fully coupled model CATHY in combination with the synthetic v-tilted catchment example of ~1 km length and assimilated piezometric head and water level data. They found that the combination of both data types gave the best predictions. This different conclusion (compared to *Camporese et al.* [2009]) might be related to the different algorithms and updating strategies used in the different studies. These studies with the assimilation of discharge data were all synthetic and linked to the reach scale. However, in practice, the applicability at the catchment scale would also be possible and even be more promising, as real-time predictions would be more relevant for larger scales. The studies with these integrated models could also be extended to include more complex interactions between river and aquifer including heterogeneous riverbeds, but this was not subject to study yet.

Another data type, relevant for studies on stream-aquifer interaction, is stream stage. Radar altimetry can obtain stream stage. As explained before in this paper, currently radar altimetry is only possible for broad rivers (with the exception of CryoSat2), and the low temporal frequency of information only makes applications at the very large catchment scale possible. The following examples for assimilation of radar altimetry data were therefore on the large catchment scale of 10^5–10^6 km^2. *Pereira-Cardenal et al.* [2011] assimilated radar altimetry data from ERS2 and Envisat by EnKF and found a considerable model improvement for a historical testing period. *Michailovsky et al.* [2013] assimilated radar altimetry data for the Brahmaputra River in Southern Asia with the extended Kalman filter. *Michailovsky and Bauer-Gottwein* [2014] applied a similar methodology for the Zambezi River. Assimilation of river stage information from altimetry is now limited to the large catchment scale, but a higher spatial and temporal resolution would allow applications at the smaller basin scale in the future. River stage measurements can also be assimilated and be useful for even smaller scales like the reach scale. However, such applications are not yet common in the scientific literature.

In the surface hydrology literature, data assimilation approaches were also used to improve predictions of rainfall-runoff models that include a groundwater component. However, river-groundwater interactions are not explicitly modeled in these simulation codes, and the main focus is on improving river discharge predictions. One example is the work of *Lee et al.* [2011] where soil moisture and river discharge data are both assimilated in the Sacramento model [*Burnash et al.*, 1973] using a variational data assimilation approach. Another example is the synthetic study by *Xie and Zhang* [2010] to assimilate the same data types and evapotranspiration data (with EnKF) in the Soil and Water Assessment Tool model [*Gassman et al.*, 2007] using EnKF.

We showed that river-groundwater models can be constrained with sequential DA assimilating river-aquifer head differences, river discharge, river stage, and/or temperature data. Further interesting data for calibration of river-groundwater models are data we presented before in section 2.1, such as, for example, stream-aquifer exchange fluxes, as measured by seepage meter, infiltrometer, or environmental tracers. These data are also suited for calibrating heterogeneous riverbeds at the hyporheic scale of 10^0–10^1 m.

In general, sequential data assimilation methods are suited and flexible to estimate model parameters at different scales, but the measurement data have to be informative about a particular scale. Consequently, the hyporheic scale requires many small-scale measurement data for model calibration. Although at this scale parameter estimation and data assimilation might seem of less interest, they can be important for process understanding. Data assimilation procedures can consider different uncertainty sources simultaneously and could allow at this scale for better disentangling uncertainty related to parameter values and model structure. On the other hand, at the large scale (e.g., catchment scale or even on a "continental scale") it is important to assimilate measurement data that exhaustively cover the area of interest or have a strong integrative nature. High-quality remote sensing data and river discharge data from many gauging stations would be very informative at those scales. Only a high-density network of in situ observations, combined with good quality remote sensing data, would allow getting more insight on the role of riverbeds for the exchange of water between rivers and aquifers at those scales. A limitation of sequential DA methods is that a large ensemble is required to approximate the prior and posterior probability density functions of the unknown states and parameters correctly. If the ensemble is too small, the uncertainty will be underestimated over time. This can partly be counterbalanced by methods like localization and inflation, which allow also applications with smaller ensembles.

To develop targeted and efficient field campaigns, inverse approaches can be used to identify key observation data. For example, *Brunner et al.* [2012] combined pareto methods with linear approaches to calculate predictive uncertainty as well as parameter identifiability. The linear approaches employed allow identifying the data worth of observations under consideration of their measurement accuracy, even before the actual measurement is carried out. Data worth in this context means the potential of an observational data type or data point to reduce the uncertainty of a prediction of interest. An example of the application of linear methods is provided by *Schilling et al.* [2014], who quantified data worth of tree rings (used as a proxy for evapotranspiration) in a model simulating the feedback between river-groundwater interactions and vegetation.

3.2. Computational Power

Computational power continues to increase rapidly, and the computational power available through grid or cloud-computing approaches and the parallelization of numerical models are bringing environmental modeling and uncertainty assessment to an entirely new level [*Renard et al.*, 2009]. Physically based models such as ParFlow (PARallel FLOW) are now fully parallelized. *Kollet et al.* [2010] used ParFlow to simulate an area of 1000 km^2 with more than 8 billion cells. The model was run on an IBM Blue-Gene supercomputer with a total of 294,912 processors and 144 TB of memory. Such large-scale modeling efforts continue to be expanded. For example, *Maxwell et al.* [2015] used ParFlow to simulate groundwater and surface water processes across most of the continental United States.

Inverse approaches such as BeoPEST available on the PEST homepage (www.pesthomepage.org) support two communication protocols (TCP/IP and MPI) to communicate between the master model and the slaves. Given that model calibration and uncertainty analysis typically require hundreds or thousands of model runs, the distribution of these computationally demanding tasks to multiple processors allows for the calibration of complex and highly parameterized models.

Cloud-computing technology provides an interesting alternative to the acquisition of a computer cluster. One of the first applications for cloud computing in hydrogeological modeling was published by *Hunt et al.* [2010]. They provided a good overview of the types and services of cloud computing and discussed some of the commercially available resources and point out that through cloud computing the user has virtually unlimited access to computing power. *Kurtz et al.* [2017] presented a cloud-based modeling system that integrates real-time data acquisition, physically based modeling of surface, and groundwater flow using HydroGeoSphere combined with data assimilation for real-time decisions on water management.

4. Discussion and Prognosis

This paper has reviewed recent advances in characterizing and modeling river and groundwater interactions and has described emerging field and modeling based approaches. Several models have been developed based on the *Freeze and Harlan* [1969] blueprint. The original blueprint presented a vision that was exclusively hydraulic in nature. Today, current and emerging challenges show that there is a myriad of questions, problems, and challenges that will lead to an evolution in the original blueprint. These include, but are not limited to, ecological and water quality questions. Different questions demand different answers. Different answers require different methodologies that must be employed at different scales. There are many emerging tools and approaches that are now available and ready to be put into widespread practice. We do not contend that every tool should be used all the time. However, awareness, familiarity, and open mind to the potential benefits of the range of advanced approaches now available for measuring, conceptualizing, understanding, and predicting river-groundwater interactions afford new and exciting possibilities that were not even conceived of a decade ago. These approaches will, in turn, lead to the development of the next generation of approaches that continue to advance this discipline of hydrologic science.

We offer some reflections and prospects about science, management, and policy that relate to this discipline of hydrologic science. These include, but are not limited to, the following:

1. Understanding the implications of different data types and resolution: Hydrologic decision making is fundamentally about understanding the likelihood (or risk) that something bad may happen. A better understanding of uncertainty and how it can be reduced by introducing different data types and at different spatial and temporal resolution will be critical in assessing the benefit-cost ratio of collecting different data at different scales. Given financial constraints, an ability to better define data types that are needed to make robust predictions to answer different questions at different scales will rely on better understanding how using different data types and resolution can reduce uncertainty and ultimately help us to make better predictions. This is important because many of the tools and techniques discussed in this review are new and will not easily be employed in practice unless the benefits are clearly quantified and understood. Understanding how different data types and their resolution relate to prediction uncertainty and

outcomes is of paramount importance and will critically influence the choice of both conceptual and numerical model simplicity-complexity.

2. Instrumented field sites: We need a series of highly equipped and long-term sites where river-groundwater interaction is investigated, ideally in different climatic regions, so that researchers from different universities and institutes could join efforts to understand river-groundwater interactions better. This would allow us to develop and obtain international high-resolution spatial and temporal data sets. In our view, sites that only focus on hydrological, or hydrogeological or ecological parameters are not sufficient for a thorough understanding. Similarly, longer-term longitudinal measurements and studies are also required. Often the funding involved to establish highly equipped and long-term sites is large and shared sites funded by different institutions and agencies may assist. Hydrological sites exist and are becoming more popular (e.g., CZO sites in the U.S. and TERENO sites in Germany). These new sites could be added to other programs such as the Long Term Ecological Research (LTER) sites (https://lternet.edu). Although river-groundwater interaction is associated with large water, energy, and solute fluxes between compartments in a special and sensitive ecosystem, river-groundwater interaction is, in general, not the main focus at those sites. Integrating LTER work with nutrient programs like "*The Lotic Intersite Nitrogen Experiments*" [*LINX collaborators*, 2014] is an example of successful ecological research collaboration and provides an important opportunity to develop interdisciplinary research collaboration in many areas, including hydroecological research.
3. Model development and improvement: It was indicated that physically based models for the interaction between river and groundwater are of great interest to advance science. Increasing computer power allows one to simulate these processes at a higher spatial and temporal resolution and to do rigorous quantitative uncertainty analysis. Physically based hydrological models can to a certain extent account for processes occurring at scales smaller than the grid scale. An example is preferential flow which can be handled without an explicit representation of the preferential flow network. However, the role of chemical and biological processes in controlling streambed permeability, and hence the interaction between rivers and groundwater, is not well captured by most models. Neither is the role of erosion and sedimentation events which also influence the permeability of the riverbeds. It might be important to capture these processes with the models, but these processes are not always important, and it is difficult to know how important they are. This will depend on the nature of the problem being considered and the associated spatiotemporal scales. We argue that for model development and improvement field sites with dense observation networks are of vital importance and that geostatistics or model-data fusion techniques like ensemble Kalman filter can help in this process.
4. Integrating models and data: This review focussed on integrating models and data. To do this, it is also important to improve the representation of processes at the stream-aquifer interface. Inverse modeling or data assimilation can also detect systematic deviations between model predictions and measured values. Systematic deviations could, for example, be related to specific conditions like flood events. The detection of such systematic deviations could be used as a feedback loop to improve models and include new processes. It is of special interest if certain systematic deviations are repeatedly found at different highly equipped sites that provide observation data across the different spatial scales. In this context, it is important that computational power increases rapidly and we have access to unprecedented types and quantity of data. This will allow the integration of additional data types and in larger quantities into models and at a higher temporal and spatial resolution. This integration of data into models also requires improved algorithms for multivariate data assimilation which can handle better non-Gaussian measurement data and are better at simultaneously handling multiple data types.
5. Management and policy drivers for next generation science: Current management and policy issues including, but not limited to, the water-food-energy-environment nexus, impacts of climate change on water resources, impacts of population growth on water requirements, water quality and health, environmental and ecological impacts of water abstraction, coal seam and shale gas and hydraulic fracturing, mining and energy, and nuclear waste disposal demand interdisciplinary approaches. They also demand strong management and policy underpinned by rigorous science. These contemporary and pressing societal issues demand new answers to new questions, and they demand new scientific approaches. More specifically, consider two examples that were illustrated in Figure 1, namely, drinking water quality (contamination) and environmental flow regimes. Some jurisdictions require that the vulnerability of drinking water sources to contamination be determined. When the source is surface water, it ultimately

requires that flow paths of groundwater entering the stream be known, since groundwater contaminants could enter the stream. Identifying the origin of groundwater entering the stream, linked to potential sources of groundwater contamination, is a challenging issue. Environmental flow regimes are another pressing matter that require sophisticated attention. Because base flow can represent a significant portion of the total flow to a stream (reaching 100% during drought), groundwater quantity and quality are very important for the viability of ecosystems in streams. The concept of environmental flow regimes extends well beyond the amount of water that flows in a river system or a minimum flow required to preserve ecosystem functions. An environmental flow regime encompasses the entire flow system and its spatiotemporal patterns. This includes the frequency and magnitude of flows as well as how long flow lasts. This understanding underpins river ecosystem health. The advances proposed here will be required to correctly define, understand, and predict environmental flow regimes as well as improve predictions of the impact of variations in groundwater quality and quantity on the health of river ecosystems. Water quality/contamination and environmental flow regimes are just two such examples where the approaches described in this paper are likely to have interesting and important applications. There are many others. New emerging management and policy issues require the latest scientific advances, and others not yet conceived, to solve them. Robust policy, management, regulation, and compliance cannot be achieved without such scientific developments and application.

This paper has reviewed recent advances in characterizing streambeds to improve the integrated simulation of surface and groundwater flow and has described emerging field and modeling-based approaches. It has demonstrated that there are many new techniques available for characterizing streambeds and modeling surface water groundwater exchanges. Raising awareness of these methods is a necessary precursor for applying them in practice and future research. What is abundantly clear from this review is that there are many tools and approaches—many that are currently not in widespread use—that are available and ready to be put into practice. This echoes views by others [e.g., *Simmons et al.*, 2012]. Our toolbox is filled with exciting tools that are both interesting and important and that will be critical for advancing both hydrologic research and application. Determining when and how to use these tools and approaches will depend on key matters including the question to be solved and the nature and scale of the problem. This will require careful consideration on a case by case basis. It is difficult to offer generalized solutions. Let us experiment bravely and boldly with all the tools in our toolbox. This is sure to help advance hydrologic science and practice, reduce what appears to be a growing gap between them [*Simmons et al.*, 2012], and ultimately forge new and exciting research frontiers.

4.1. Tutorial 1: Integrated Surface and Subsurface Hydrologic Model

The blueprint presented by *Freeze and Harlan* [1969] proposed to represent water transmission and storage in a hydrologic system by a distributed system model. Instead of relying on separate models that decouple surface water flow and groundwater flow, as was done at that time, they suggested representing the various components of the water cycle shown in Figure T1.1 in a single model, by simultaneously solving surface water and groundwater flow. Examples of such models include CATHY [*Paniconi et al.*, 2003], HydroGeoSphere [*Therrien et al.*, 2009; *Aquanty*, 2016], PARFLOW [*Kollet and Maxwell*, 2006], OpenGeoSys [*Kolditz et al.*, 2012], or MIKE SHE [*Havnø et al.*, 2005; *Refsgaard and Storm*, 1995] which is now further developed by DHI-WASI (www.wasy.de/).

This tutorial presents the main components of a typical ISSHM by using the HydroGeoSphere model as an example. The continuity equations for subsurface and surface flow, as well as the relationships between water fluxes and energy gradient, are presented.

Similar to most other ISSHMs, the continuity equation used in HydroGeoSphere to represent variably saturated groundwater flow in a porous medium (subsurface) is the 3-D Richards' equation

$$-\nabla \cdot q + \Gamma_o = \frac{\partial \theta_s S_w}{\partial t}$$

where Γ_o represents the volumetric flux of water exchange per unit volume ($L^3\ L^{-3}\ T^{-1}$) between the surface and the subsurface, θ_s is the porous medium porosity ($L^3\ L^{-3}$), and S_w is its water saturation ($\mathrm{L}^3\ \mathrm{L}^{-3}$). Darcy's law gives the groundwater flux q ($L\ T^{-1}$) according to

$$q = -K \cdot k_r \nabla(\psi + z)$$

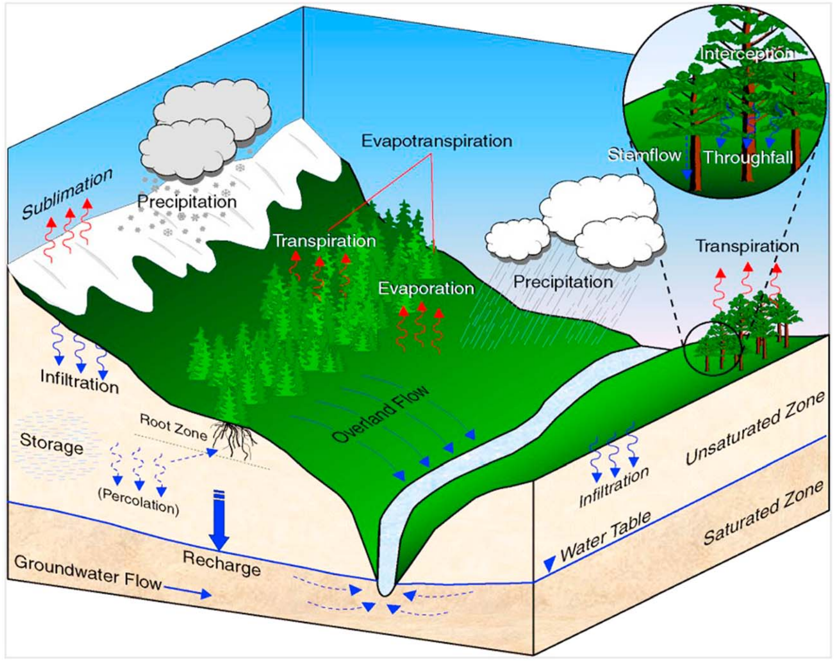

Figure T1.1. Components of the water cycle considered in the Freeze and Harlan blueprint [the figure is taken from *Jyrkama* [2003]].

where K is the hydraulic conductivity of the porous medium ($L\ T^{-1}$), k_r is its relative permeability ($-$), and ψ and z are the subsurface pressure head (L) and elevation head (L), respectively.

Surface, or overland flow, is described by the following 2-D diffusion wave approximation of the St. Venant equation

$$-\nabla \cdot d_o q_o + d_o \Gamma_o = \frac{\partial \phi d_o}{\partial t}$$

where d_o is the water depth at the surface (L), ϕ is an equivalent saturation function ($-$) for the surface that can account for the presence of microtopography and flow obstructions at a scale smaller than the discretization scale, and q_o is the surface water flux ($L\ T^{-1}$) given by

$$q_o = -\frac{d_o^{2/3}}{n\Phi^{1/2}} \cdot k_{ro} \nabla (d_o + z_o)$$

where n is a surface roughness coefficient ($L^{-1/3}\ T$); Φ is the surface water gradient ($-$); k_{ro} is an equivalent relative permeability function ($-$) that, similarly to function ϕ, can account for the presence of microtopography and flow obstructions; and z_o is ground surface elevation (L).

In HydroGeoSphere, the control volume finite element method is used for the 3-D discretization of the subsurface flow equation and the 2-D discretization of the surface flow equation. A 3-D and a 2-D mesh are therefore both generated. The 2-D mesh representing the surface domain corresponds exactly to the top of the 3-D mesh, therefore creating nodes that belong to both the surface and the subsurface flow domains (dual nodes), as illustrated in Figure T1.2.

The 2-D and 3-D flow equations are solved simultaneously. Both equations are nonlinear, and the Newton-Raphson linearization technique is used for the solution. Fluid exchange Γ_o between the surface and subsurface domain is computed at the dual nodes during the flow solution. Fluid exchange can be represented by assuming continuity of potential at the dual nodes, with the water depth d_o being equal to the subsurface pressure head ψ. Another representation that does not rely on that assumption represents fluid exchange with the following equation

$$d_o \Gamma_o = K_{SO} k_{rso} (\psi - d_o)$$

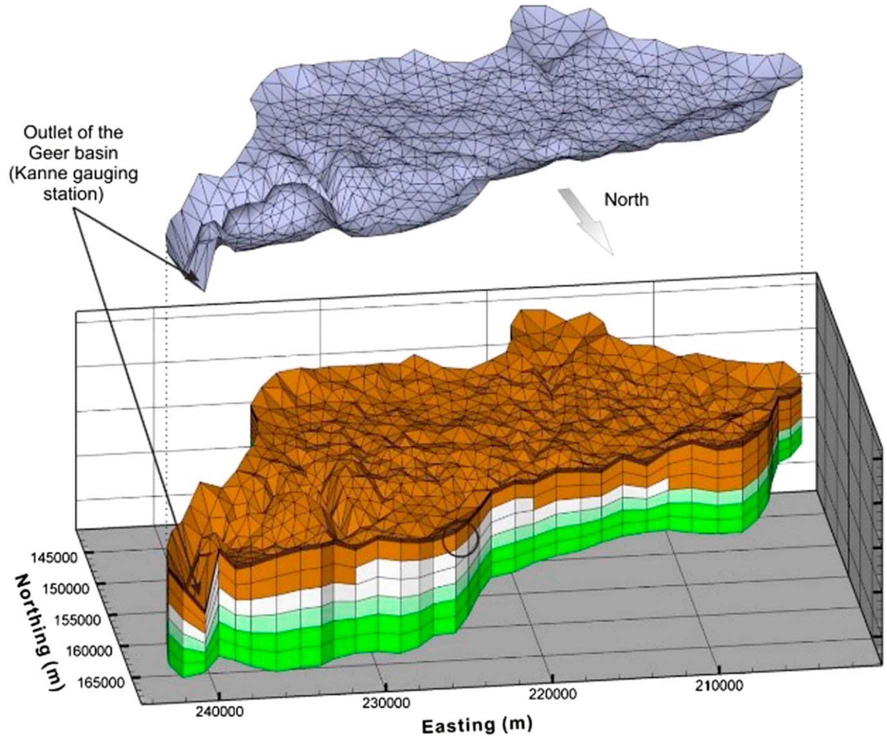

Figure T1.2. Illustration of a discretized river-groundwater model for the 480 km^2 Geer Basin, Belgium (Figure taken from *Goderniaux et al.* [2009]). The surface flow domain is discretized in 2-D with triangular elements, and the subsurface flow domain is discretized in 3-D with triangular prisms (6-node elements). The 2-D domain is shown separately here, but it corresponds exactly to the top of the 3-D subsurface mesh.

where K_{SO} is the hydraulic conductivity of the interface between the surface and subsurface ($L\,T^{-1}$) and k_{rso} is the relative permeability of that interface (−).

Because of the surface flow continuity equation used in HydroGeoSphere, which requires that the whole surface is discretized with 2-D elements, there is no need to define a priori the surface drainage network. If the surface topography is discretized with enough precision and if appropriate surface flow properties (surface roughness) are used to represent channels or streams, the solution of the surface flow equation during the simulation can satisfactorily reproduce the drainage network (as illustrated in Figure T1.3). Other ISSHMs use different continuity equations for surface flow, which leads to different discretization procedures. For example, the CATHY model [*Paniconi et al.*, 2003] couples the 3-D Richards' equation for subsurface flow to a 1-D diffusive wave approximation to surface flow and it requires the definition of a drainage network using one-dimensional coordinates to represent single hillslopes or channels.

In a numerical model such as HydroGeoSphere, it is possible to define spatially variable properties for the surface and subsurface elements, which allows representation of heterogeneous streambeds [*Brunner and Simmons*, 2012]. However, the representation of small-scale streambed heterogeneities (i.e., the hyporheic scale) requires very fine spatial discretization, which can generate models with a very large number of elements and nodes. The model run times can become very large such that they could represent a computational hurdle to represent small-scale streambed heterogeneity.

4.2. Tutorial 2: Geostatistics and River-Groundwater Interactions

All geostatistical methods treat the variability of a given physical property as a stochastic process [*Matheron*, 1962; *Journel*, 1989; *Chiles and Delfiner*, 2012]. Consider variable $Z(\mathbf{x})$, which is a property varying in space as a function of position vector $\mathbf{x}$. Variable Z can be continuous and represent the permeability, porosity, or thickness of a streambed. It can also be discrete and represent categorical data such as sediment type or the presence or absence of streambed clogging. Variable Z can also represent a vectorial or tensorial quantity such as the hydraulic conductivity tensor or a parameterized grain-size distribution. Usually, $Z(\mathbf{x})$ can only be measured at a discrete, and often small, number of locations x_i with $i \in \{1, \cdots, n\}$. Raw measurements therefore consist of n values of Z: $Z_i = Z(x_i)$ with $i \in \{1, \cdots, n\}$.

A fundamental assumption in geostatistics is to represent property Z as a random function instead of a deterministic function. A random function is fully described by the joint statistical distribution of values of $Z(\mathbf{x})$ at any locations. When this distribution is defined, one can derive from it the probability of occurrence of any value of Z at any location and conditioned to all measured values. In practice, most geostatistical methods represent the joint distribution as a multi-Gaussian distribution function, which is the Gaussian distribution function extended to multiple dimensions to account for any number of joint variables. The motivation for using a multi-Gaussian distribution function is that the resulting equations are analytically tractable and their parameterization only requires the mean value and a covariance model.

It is straightforward to estimate the mean value and covariance model from field measurements Z_i using statistical techniques such as maximum likelihood or the method of moments. Having estimated these parameters, one can then use kriging to represent the spatial variability of the expected value of $Z(\mathbf{x})$ at any location. Kriging produces smoothly varying maps that honor measurements and minimize the expected value of the estimation error at any spatial location. However, those maps represent only the variability of the expected value of $Z(\mathbf{x})$, $E(Z(\mathbf{x}))$, but do not adequately represent the spatial variability of the underlying variable $Z(\mathbf{x})$.

Techniques other than kriging are required to quantify the impact of the variability of Z on another process, for example, river-groundwater interactions, that cannot be expressed as a linear function of $Z(\mathbf{x})$. The most common techniques include Monte Carlo simulations and stochastic simulations [*Delhomme*, 1979]. Instead of generating a single map that represents the expected value of $Z(\mathbf{x})$ at any location, these techniques aim to generate an ensemble of possible realizations $Z_\omega(\mathbf{x})$, with ω being an index over a (possibly infinite) number of maps that can be generated by the statistical random function. These realizations are conditioned to point measurements, and they adequately represent the spatial variability of the property of interest, or more precisely the spatial variability of the random process whose parameters have been inferred from the data. These maps are not expected to be accurate locally, but they display a structure that is consistent with the statistics derived from the data.

In the 1990s, several authors pointed out that spatial structures generated from a multi-Gaussian statistical distribution have some systematic features that may not realistically represent the connectivity of subsurface materials [e.g., *Gómez-Hernández and Wen*, 1998]. A wide range of alternative geostatistical models was therefore developed to address this issue, including the multiple-point statistics approach that radically changed the underlying principles of geostatistics. The main ideas behind multiple-point statistics were (1) to abandon the multi-Gaussian framework and use a nonparametric approach to increase flexibility in the type of statistical distributions, (2) to consider patterns from several points simultaneously (the multiple points) and abandon covariances that are limited to pairs of points, and (3) to derive the multiple point statistics from a complete training data set (the training image) instead of the limited discrete field data from a given site.

Multiple-point statistics have been used to model the topography of the Waimakariri River in New Zealand, where the training data set is the river topography measured using lidar (Figure T2.1). With the traditional geostatistical approach, the parameters of a theoretical covariance model are inferred from these measurements to model the topography. With MPS, one can directly learn the spatiotemporal patterns from the dense data set (Figure T2.1a). The user provides the training data and specifies some parameters controlling the algorithm, such as the number of neighbors, the secondary variables to describe the trends, or the maximum difference between patterns. Those parameters often have to be adjusted according to the complexity of the training image and the type of patterns to be modeled. Some recommendations are provided in *Meerschman et al.* [2013].

A practical limitation of MPS methods is that getting the training data is not always simple, especially for modeling three-dimensional subsurface heterogeneity. An alternative is to use a process-based or object-based model to generate a training data set or to use analog physical experiments in the laboratory, which is, however, not always feasible. One can also combine various modeling methods to populate 3-D domains with realistic patterns. Figure T2.2a shows an example where a 3-D hydraulic conductivity distribution was generated by stacking successive topographies modeled with MPS based on the approach of *Pirot et al.*

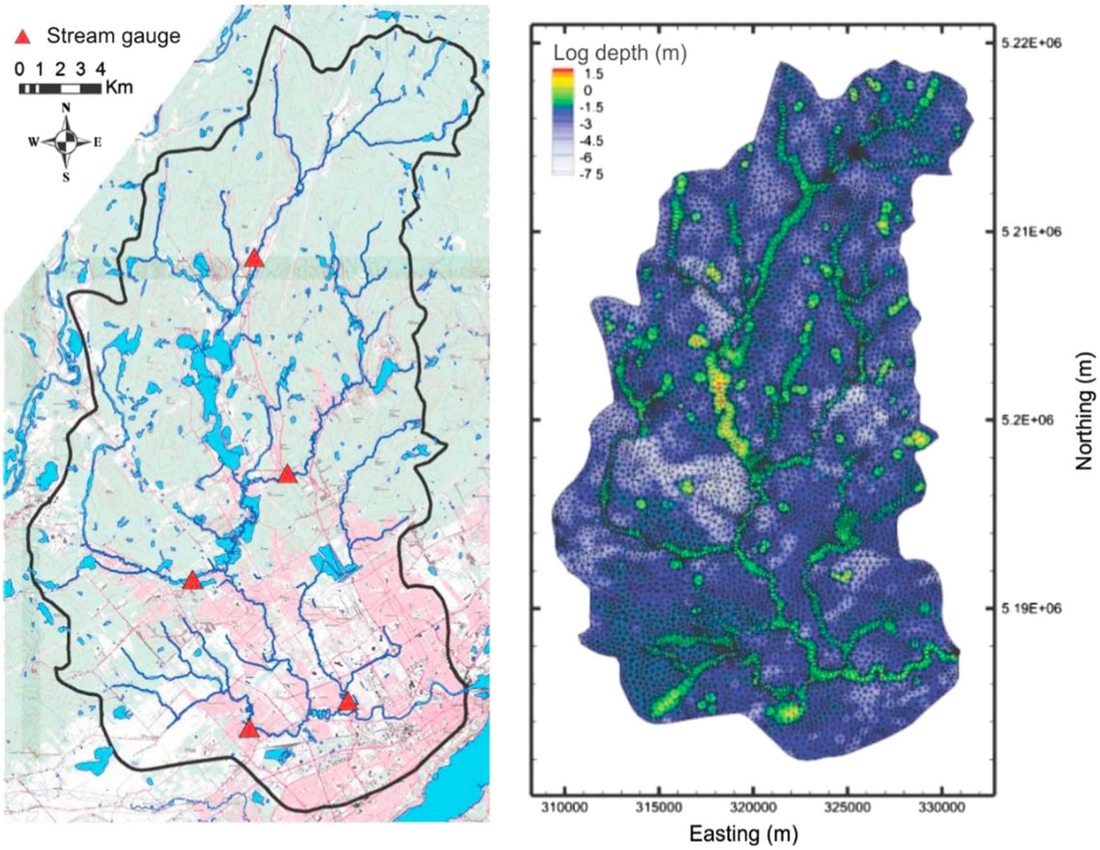

Figure T1.3. (left) Observed drainage network and (right) surface water depth (on a logarithmic scale) simulated with the HydroGeoSphere model for the Saint-Charles River catchment, Quebec, Canada (figure taken from *Cochand* [2014]).

[2014]. Additionally, geological rules for filling volumes with reasonable assumptions about the sediment grain size were specified.

The resulting patterns compare favorably with those observed on outcrops. They also contain interesting features such as cross-bedding or inclined beds, with alternating principal directions of anisotropy that influence the overall physical properties of the system and could, for example, trigger helicoidal flow [*Stauffer*, 2007; *Chiogna et al.*, 2016]. These processes could occur in streambeds and influence hyporheic flow and mixing in a manner that has yet to be studied.

Finally, because multi-Gaussian geostatistics are implicitly used in most inversion or data assimilation techniques, results of geophysical inversion, hydraulic tomography, or thermal inversion often show a multi-Gaussian spatial structure and therefore look like Figure T2.2b. These inversions cannot be used as training data sets for an MPS approach. However, different methods exist to integrate geological constraints on the spatial structure within the inversion procedure (see review by *Linde et al.* [2015]). For example, the prior distribution of parameters can be assumed to follow an MPS model and the inversion results may be more geologically realistic and potentially used as a training data set. These new methods may lead to a better understanding of the internal heterogeneity of streambeds in a first step and toward a better understanding of the impact of these structures on river-groundwater interactions in a second step.

4.3. Tutorial 3: State-of-the-Art Surface Water-Groundwater Interaction Modeling Case Study: Lehstenbach Catchment in Southeastern Germany

ISSHMs are being increasingly used to solve hydrological problems. A key outstanding issue has been how to quantify streamflow generation mechanisms. The groundwater component of streamflow, in space and time, can be estimated using tracers and hydraulic approaches, or with numerical models [*Partington et al.*, 2012]. *Partington et al.* [2011] developed a Hydraulic Mixing Cell (HMC) model and coupled it to an ISSHM. The HMC model is based on the water balance in the stream and uses the subsurface/surface fluid exchanges along the

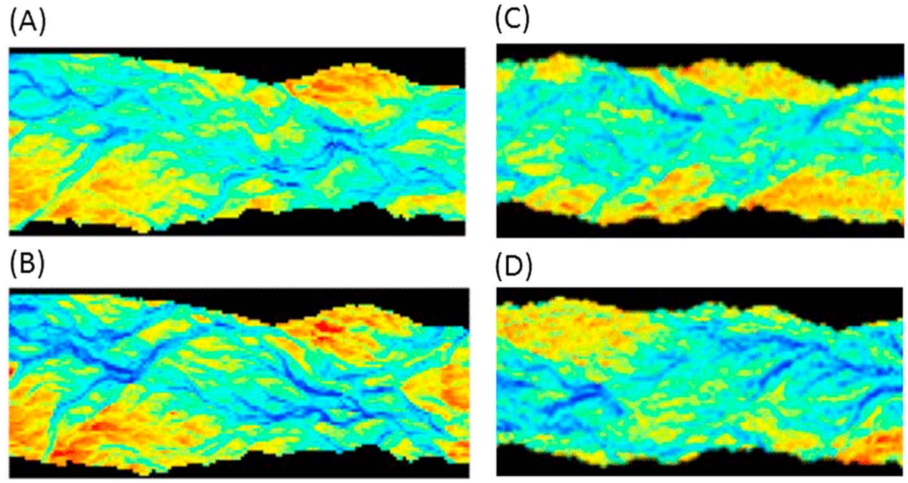

Figure T2.1. Simulation of topography using Multiple-Point Statistics (MPS]. (a and b) Waimakariri River (New Zealand) bed topography measured with lidar at two successive dates. Figures T2.1a and T2.1b are used as training images. The color represents the altitude, red are high values, and blue are low values. (c and d) Simulated successive topographies using MPS and conditional probability distributions derived from partial resampling of the two training images. The MPS algorithm uses the patterns of channels and bars that are visible in each image, as well as the complex spatial relationship between the two images, which allows realistic modeling of channel or bar migration, erosion, filling of trough, etc. (caption and images modified from *Pirot et al.* [2014]).

stream that are calculated by the ISSHM. The HMC model therefore allows the determination of groundwater flow components using only the flow solution of the ISSHM. Because the method uses only hydraulic information calculated by the ISSHM, it does not require the simulation of tracers in a solute transport model as was done in *Jones et al.* [2006].

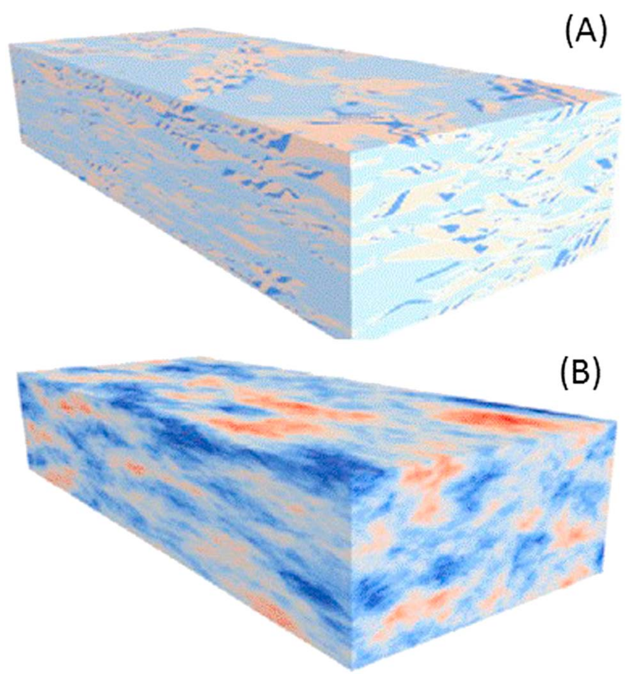

Figure T2.2. Comparison of (a) the three-dimensional heterogeneity patterns generated by the pseudo-genetic method proposed by *Pirot et al.* [2015a] with (b) a more parsimonious multiGaussian model. The color represents hydraulic conductivity values. The red color corresponds to high values and the dark blue to low values. The domain has a length of 280 m, a width of 110 m, and a thickness of 10.5 m (caption and images modified from *Pirot et al.* [2015b]).

Partington et al. [2013] applied the HMC model coupled to an ISSHM to the Lehstenbach catchment in southeastern Germany, shown in Figure T3.1 (Figure 4 of the original paper). The figure illustrates the spatial complexity in the catchment, which contains significant topographic variations that complicate the rainfall-runoff-stream generation processes. An ISSHM was applied at two contrasting scales: a smaller riparian wetland of area 210 m^2 and a larger catchment of area 4.2 km^2.

A large storm event was simulated in the catchment, and the ISSHM was employed to determine the spatial and temporal variabilities of surface saturation, exchange flux, and surface water depth prior to the storm, at the peak of the storm, and 2 days after the storm, as shown in Figure T3.2 (Figure 9 of the original paper). This figure shows the complex spatial and temporal patterns that evolve in the hydrologic response in the system and in surface water-groundwater interaction. Further, the ISSHM allows the quantitative spatial

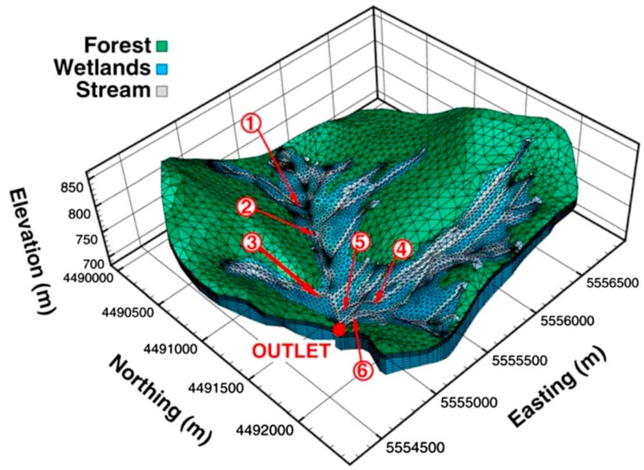

Figure T3.1. Text of the caption directly from the original publication of *Partington et al.* [2013]. Model spatial discretization of the Lehstenbach catchment and distribution of the stream, wetland, and forest areas (the *z* axis is exaggerated by a factor of 5). Model observation points are at locations 1–6 and at the outlet.

and temporal prediction of exchange fluxes, where a positive exchange flux indicates groundwater flow to the stream and a negative value indicates that the stream is losing water to the aquifer through infiltration.

Figure T3.3 (Figure 10 of the original paper) shows the hyetograph, discharge hydrographs simulated at the outlet, and the HMC fractions in surface-storage across the catchment. In the smaller-scale wetland model, complex processes were simulated using microtopographic information across the wetlands.

Groundwater discharge to the wetland surface (GW-WL) is shown in Figure T3.4 (Figure 7 of the original paper). Wetland HMC fractions at 20

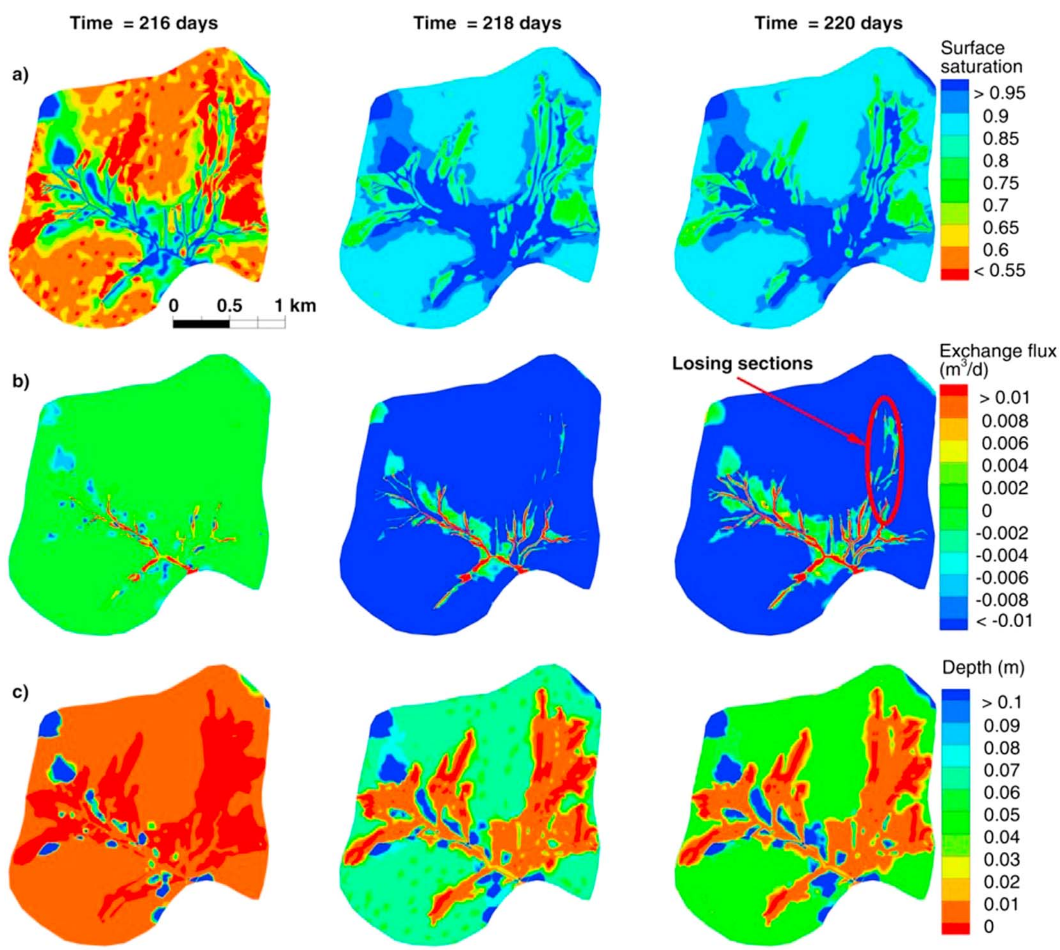

Figure T3.2. Text of the caption directly from the original publication of *Partington et al.* [2013]. (a) Simulated surface saturation, (b) exchange flux, and (c) surface water depth, before the storm, at the storm peak and 2 days after the storm peak. A losing section on the right arm of the stream is highlighted in the third frame of Figure T3.2b. Positive values of exchange flux indicate groundwater discharge to the surface, and negative values indicate infiltration of surface water to the subsurface.

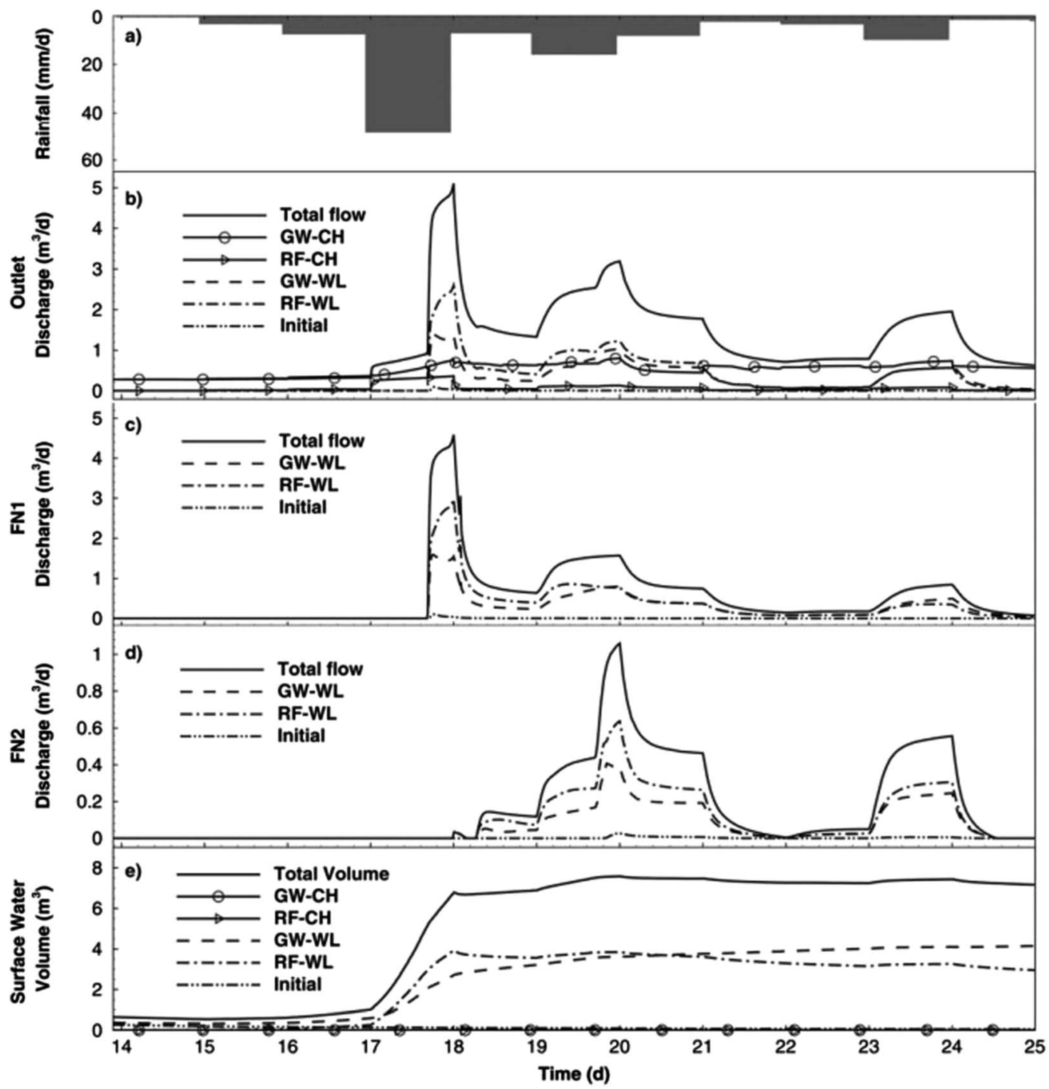

Figure T3.3. Text of the caption directly from the original publication of *Partington et al.* [2013]. (a) Hyetograph, (b) separated simulated discharge hydrographs at the outlet, and (c) the HMC fractions in surface-storage across the catchment. Note that simulated overland flow from the forest was negligible (<0.2%) in contributing to streamflow and so is not shown in Figure T3.3b.

(during the storm event) are shown. In these figures, a GW-WL fraction of 0.5 tells us that 50% of the water in the cell was generated by groundwater discharge to the wetland surface. The model results show the wetland filling and the significant component of groundwater discharge to the wetland during the storm event. In both the regional-scale catchment model and smaller wetland model, the combined use of an ISSHM together with the HMC method represents state-of-the-art modeling in surface water-groundwater interaction studies. This application illustrates the current power of ISSHM's for modeling and analyzing surface water-groundwater interactions.

ISSHMs are being increasingly used in hydrologic research, but *Liggett et al.* [2015] observed that solute transport in ISSHMs is largely unexplored. They noted that previous studies where solute transport is simulated have focused on smaller scales, simple systems, and spatial domains and have largely tended to underutilize field data sources. *Liggett et al.* [2015] simulated flow and solute transport in the Lehstenbach catchment, where high-resolution dissolved organic carbon (DOC) observations were available and provided a powerful way to analyze solute transport mechanisms. In particular, DOC transport and export from the wetland during a rainfall event was analyzed. The study included a sensitivity analysis to examine the way in which solute

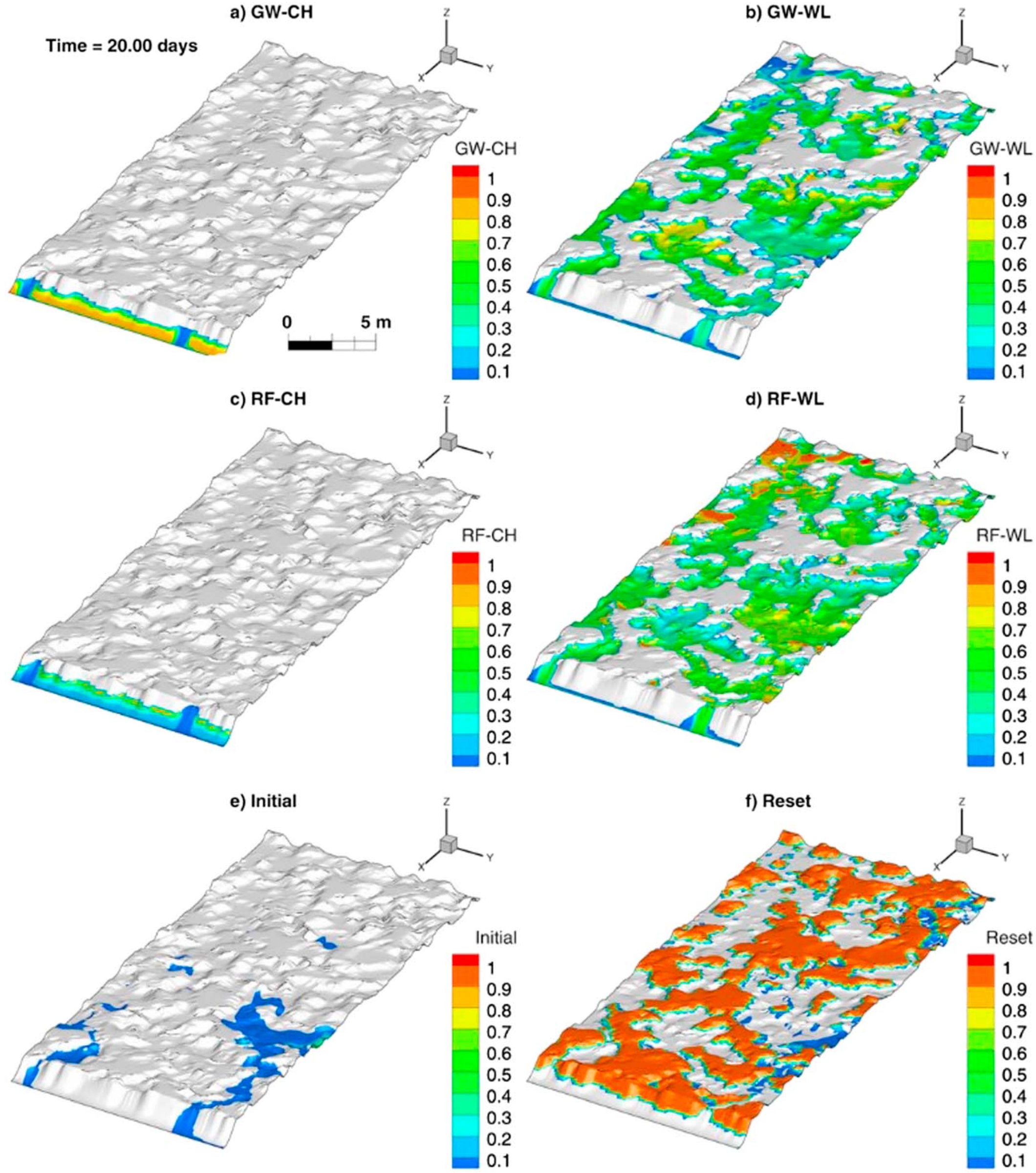

Figure T3.4. Text of the caption directly from the original publication of *Partington et al.* [2013]. Wetland HMC fractions at day 20 (during the storm event). In-stream and overland flow generating mechanisms shown are (a) groundwater discharge to the channel, (b) groundwater discharge to the wetland surface, (c) rainfall to the channel, and (d) rainfall to the wetland. (e) The remaining initial water and (f) the reset fraction for reset cells are also shown.

transport conditions across the surface-subsurface boundary influenced model results. Advective exchange only, advection plus diffusion, advection plus full mechanical dispersion, and subsurface dispersivity were included in the sensitivity analysis. Figure T3.5 (Figure 7 of the original paper) shows the simulated total DOC mass flux at the catchment outlet obtained using the various interface transport conditions and with various values of subsurface dispersion. It is clear that there is a significant influence of dispersion both across the surface-subsurface interface and from the subsurface dispersion. Results from Figure T3.5 show a wide range of solute transport behavior. This range represents a significant challenge for solute transport simulations and, in the absence of a detailed understanding of the appropriate processes at the representative scales, may lead to nonunique solute transport results.

Liggett et al. [2015] reported that the ISSHM correctly captures some, but not all observed catchment behaviors. For example, the model correctly simulates the observed solute discharge at the catchment outlet and

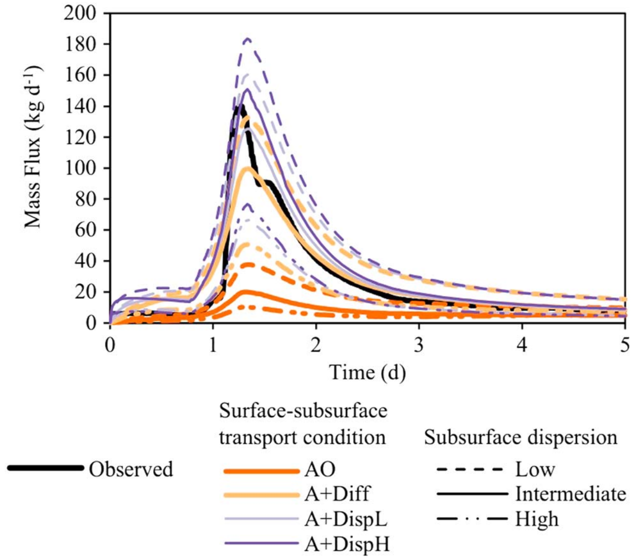

Figure T3.5. Text of the caption directly from the original publication of *Liggett et al.* [2015]. Influence of subsurface dispersion on the mass flux of total DOC at the catchment outlet.

the observed increasing discharge from wetlands that occurs with increased stream discharge. However, the slope of the concentration-discharge plots was not well represented in the model. While solute transport measurements and behavior potentially and theoretically assist with constraining model behavior and better understanding constituent physical processes (and the decomposition of the stream hydrograph), it also introduces a range of additional solute transport parameters into the analysis. These include dispersion and diffusion at the surface-subsurface interface and subsurface dispersion. Also important are the spatial patterns of the solute transport initial conditions—in this case, DOC. The initial condition for DOC concentration in the river and aquifer will be important determinants of subsequent spatial and temporal behavior of the DOC concentrations throughout the model. These represent the initial "end-member" concentrations that are subject to transport, both advection and dispersive mixing. Introducing solute transport into the simulation increases complexity, but the potential for solute transport to offer advantages for understanding and constraining both hydraulics and transport behavior in a catchment is significant. This potential will be strongly dependent on obtaining solute transport field data, at appropriate scales, for constraining and validating solute ISSHMs. Furthermore, these approaches could be useful in hydroecological studies. For example, they could be used to relate to ecosystem studies that look at biological DOC uptake (for comparisons with a model where no uptake is included).

These state-of-the-art studies are currently demonstrating the tremendous power and utility of ISSHMs in hydrologic research and for studying surface water-groundwater interaction. While it is evident that the Freeze and Harlan [1969] *"Blueprint for a physically-based, digitally-simulated hydrologic response model"* is now the basis for the latest and emerging generation of ISSHMs, it is also evident that the inclusion of solute transport in ISSHMs remains largely unexplored and poorly understood. It thus represents a key line of future research development and application inquiry.

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